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Applied Machine Learning: Module 2 (Supervised Learning, Part I)

Preamble and Review

```
In [1]: %matplotlib notebook
import numpy as np
import pandas as pd
import seaborn as sn
import matplotlib.pyplot as plt

from sklearn.model_selection import train_test_split
from sklearn.neighbors import KNeighborsClassifier

np.set_printoptions(precision=2)

fruits = pd.read_table('fruit_data_with_colors.txt')

feature_names_fruits = ['height', 'width', 'mass', 'color_score']
X_fruits = fruits[feature_names_fruits]
y_fruits = fruits['fruit_label']
target_names_fruits = ['apple', 'mandarin', 'orange', 'lemon']

X_fruits_2d = fruits[['height', 'width']]
y_fruits_2d = fruits['fruit_label']

X_train, X_test, y_train, y_test = train_test_split(X_fruits, y_fruits, random_state=0)

from sklearn.preprocessing import MinMaxScaler
scaler = MinMaxScaler()
X_train_scaled = scaler.fit_transform(X_train)
# we must apply the scaling to the test set that we computed for the training set
X_test_scaled = scaler.transform(X_test)

knn = KNeighborsClassifier(n_neighbors = 5)
knn.fit(X_train_scaled, y_train)
print('Accuracy of K-NN classifier on training set: {:.2f}'
     .format(knn.score(X_train_scaled, y_train)))
print('Accuracy of K-NN classifier on test set: {:.2f}'
     .format(knn.score(X_test_scaled, y_test)))

example_fruit = [[5.5, 2.2, 10, 0.70]]
example_fruit_scaled = scaler.transform(example_fruit)
print('Predicted fruit type for ', example_fruit, ' is ',
      target_names_fruits[knn.predict(example_fruit_scaled)[0]-1])
```

```
Accuracy of K-NN classifier on training set: 0.95
Accuracy of K-NN classifier on test set: 1.00
Predicted fruit type for  [[5.5, 2.2, 10, 0.7]]  is  mandarin
```

Datasets

```
In [2]: from sklearn.datasets import make_classification, make_blobs
from matplotlib.colors import ListedColormap
from sklearn.datasets import load_breast_cancer
from adspy_shared_utilities import load_crime_dataset

cmap_bold = ListedColormap(['#FFFF00', '#00FF00', '#0000FF','#000000'])

# synthetic dataset for simple regression
from sklearn.datasets import make_regression
plt.figure()
plt.title('Sample regression problem with one input variable')
X_R1, y_R1 = make_regression(n_samples = 100, n_features=1,
                             n_informative=1, bias = 150.0,
                             noise = 30, random_state=0)
plt.scatter(X_R1, y_R1, marker= 'o', s=50)
plt.show()

# synthetic dataset for more complex regression
from sklearn.datasets import make_friedman1
plt.figure()
plt.title('Complex regression problem with one input variable')
X_F1, y_F1 = make_friedman1(n_samples = 100,
                            n_features = 7, random_state=0)

plt.scatter(X_F1[:, 2], y_F1, marker= 'o', s=50)
plt.show()

# synthetic dataset for classification (binary)
plt.figure()
plt.title('Sample binary classification problem with two informative features')
X_C2, y_C2 = make_classification(n_samples = 100, n_features=2,
                                 n_redundant=0, n_informative=2,
                                 n_clusters_per_class=1, flip_y = 0.1,
                                 class_sep = 0.5, random_state=0)
plt.scatter(X_C2[:, 0], X_C2[:, 1], c=y_C2,
            marker= 'o', s=50, cmap=cmap_bold)
plt.show()
```

```
# more difficult synthetic dataset for classification (binary)
# with classes that are not linearly separable
X_D2, y_D2 = make_blobs(n_samples = 100, n_features = 2, centers = 8,
                        cluster_std = 1.3, random_state = 4)
y_D2 = y_D2 % 2
plt.figure()
plt.title('Sample binary classification problem with non-linearly separable classes')
plt.scatter(X_D2[:,0], X_D2[:,1], c=y_D2,
            marker= 'o', s=50, cmap=cmap_bold)
plt.show()

# Breast cancer dataset for classification
cancer = load_breast_cancer()
(X_cancer, y_cancer) = load_breast_cancer(return_X_y = True)

# Communities and Crime dataset
(X_crime, y_crime) = load_crime_dataset()
```

Figure 1

Sample regression problem with one input variable

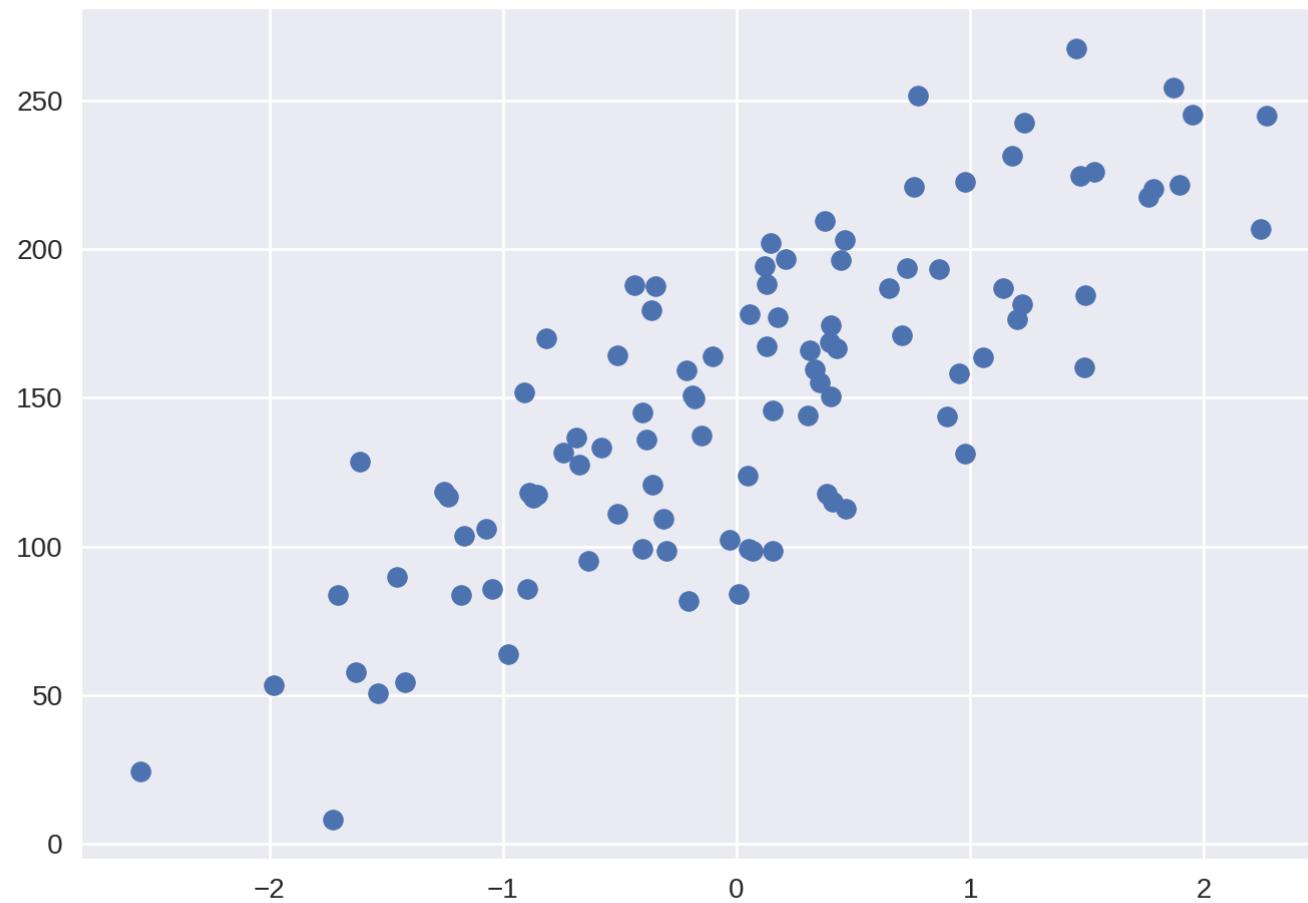


Figure 2

Complex regression problem with one input variable

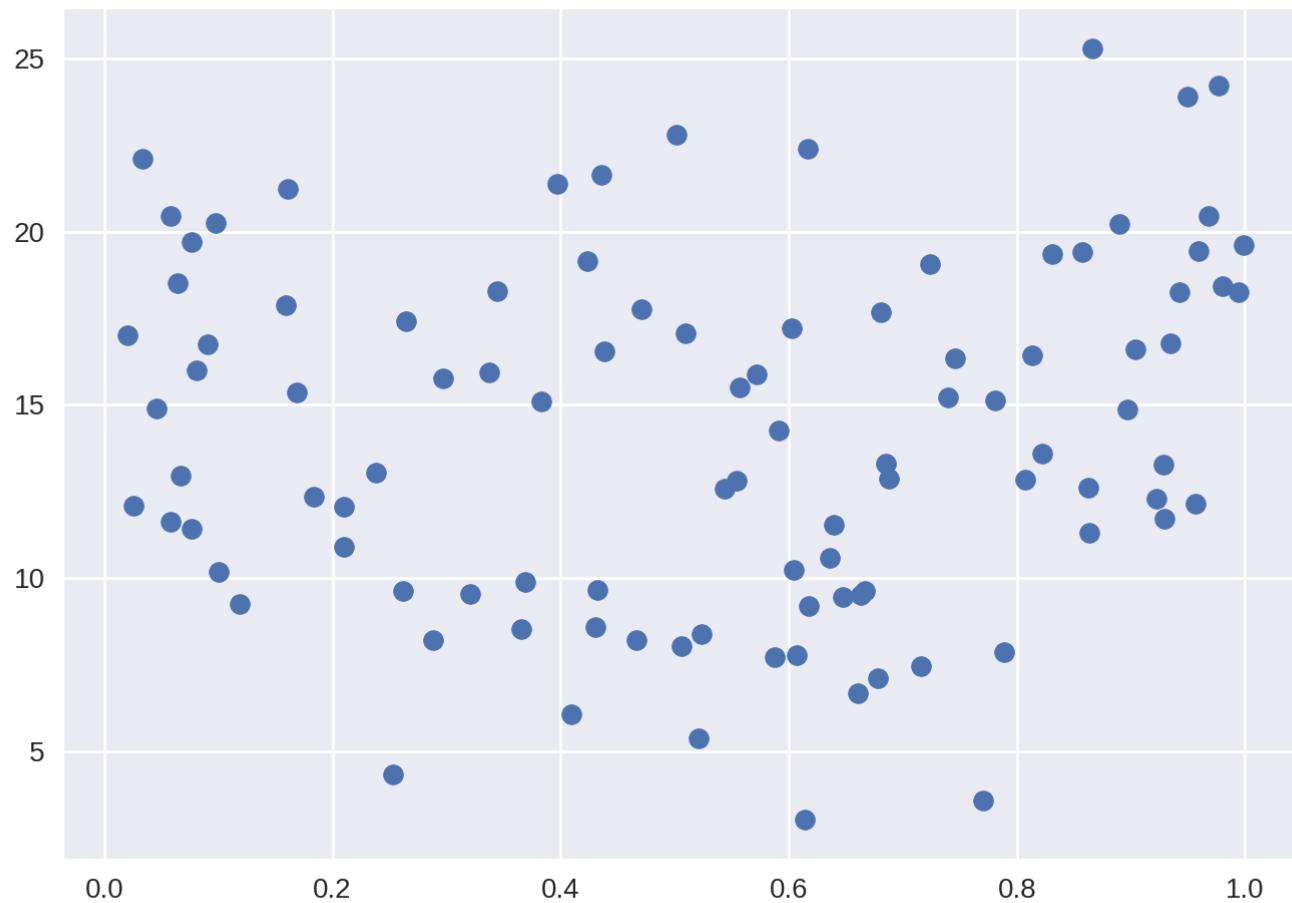


Figure 3

Sample binary classification problem with two informative features

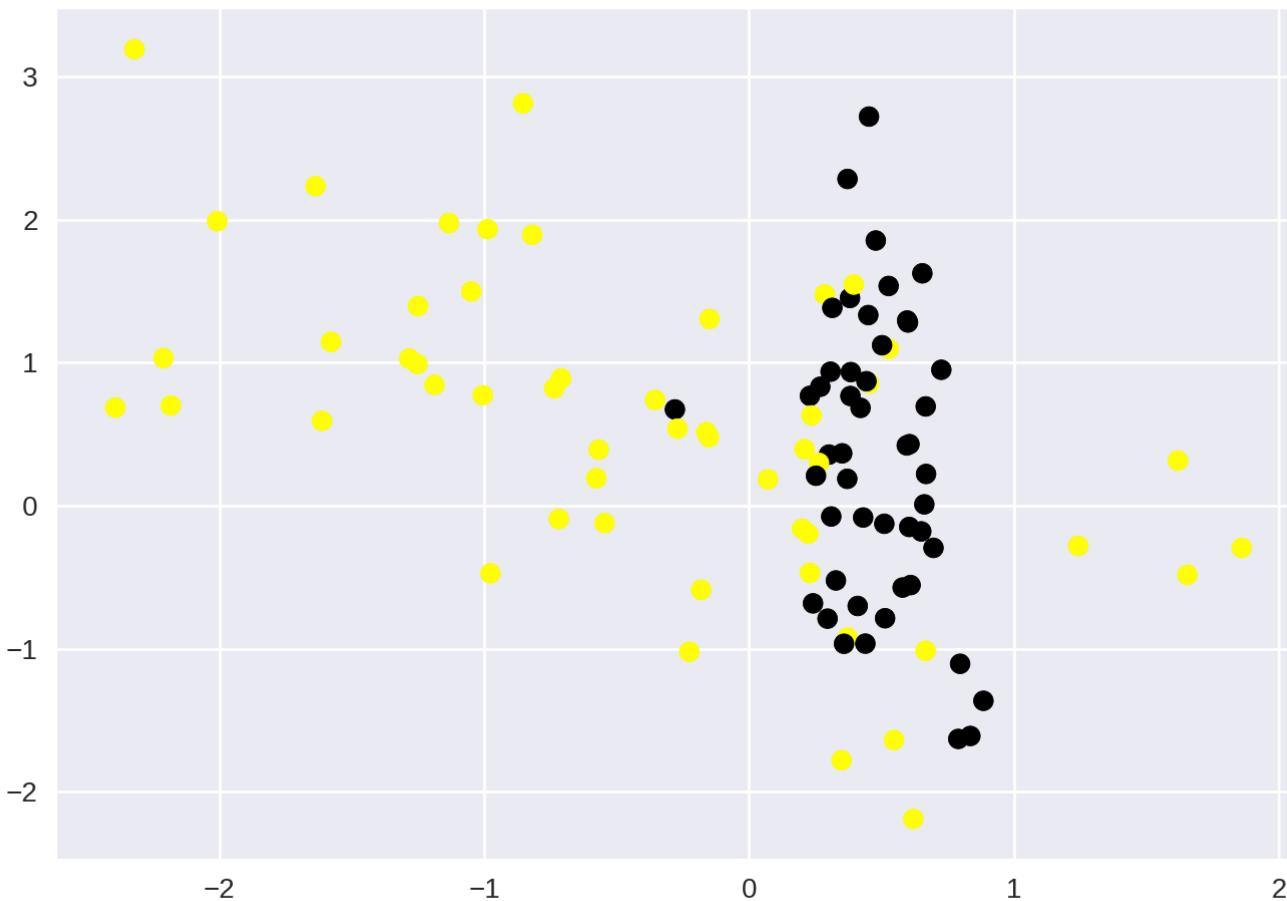
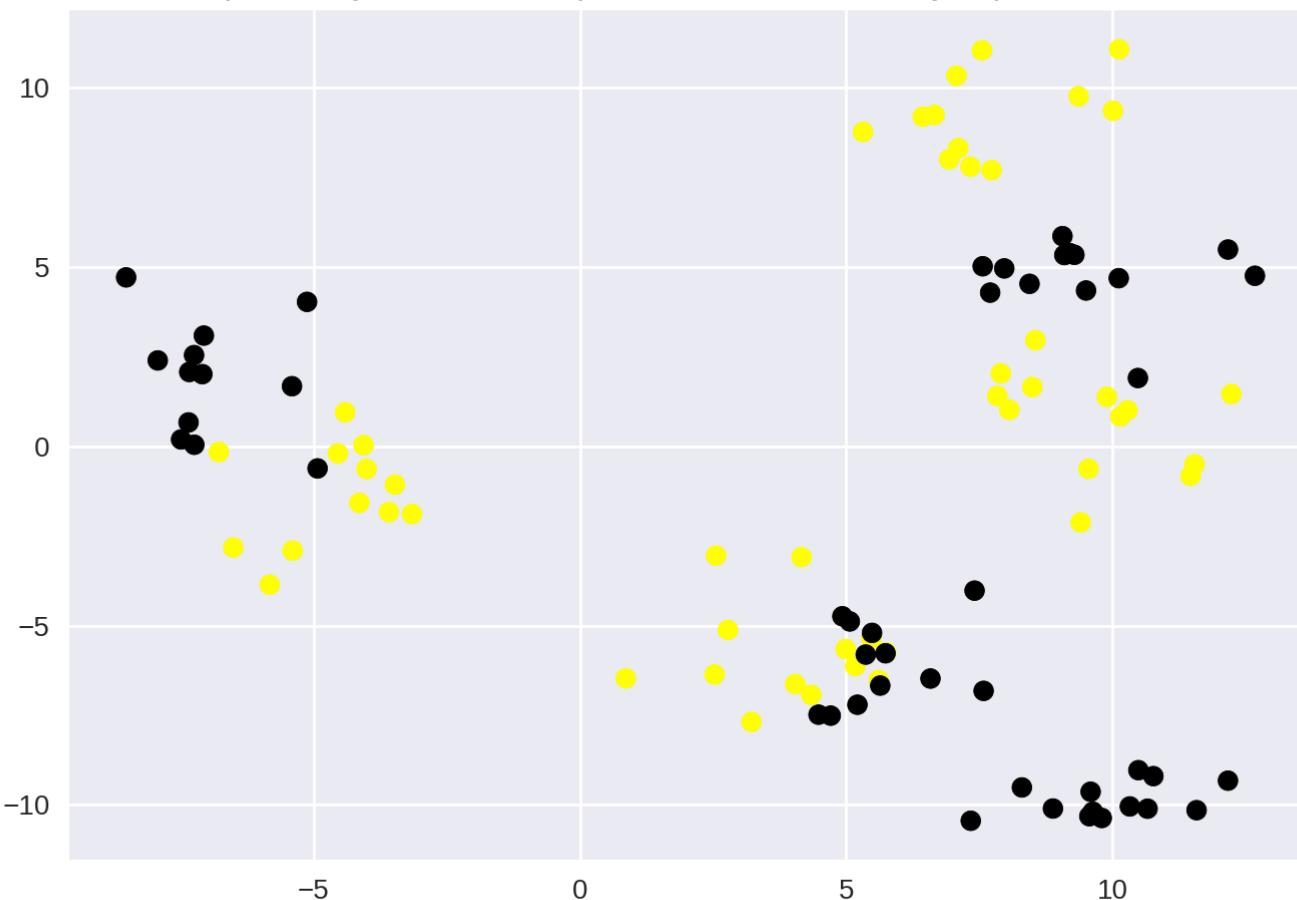


Figure 4

Sample binary classification problem with non-linearly separable classes



K-Nearest Neighbors

Classification

```
In [3]: from adspy_shared_utilities import plot_two_class_knn

X_train, X_test, y_train, y_test = train_test_split(X_C2, y_C2,
                                                random_state=0)

plot_two_class_knn(X_train, y_train, 1, 'uniform', X_test, y_test)
plot_two_class_knn(X_train, y_train, 3, 'uniform', X_test, y_test)
plot_two_class_knn(X_train, y_train, 11, 'uniform', X_test, y_test)
```

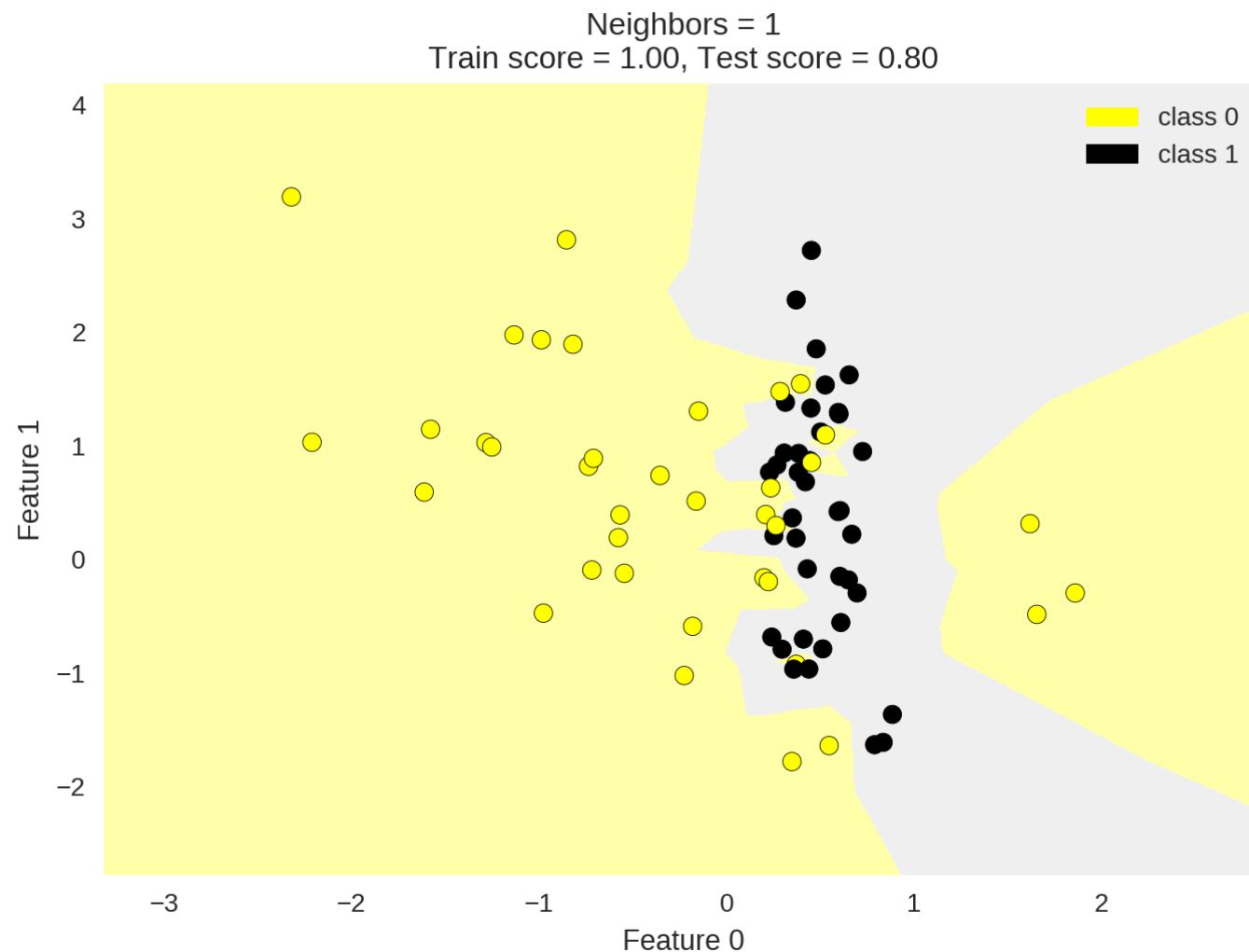
Figure 5

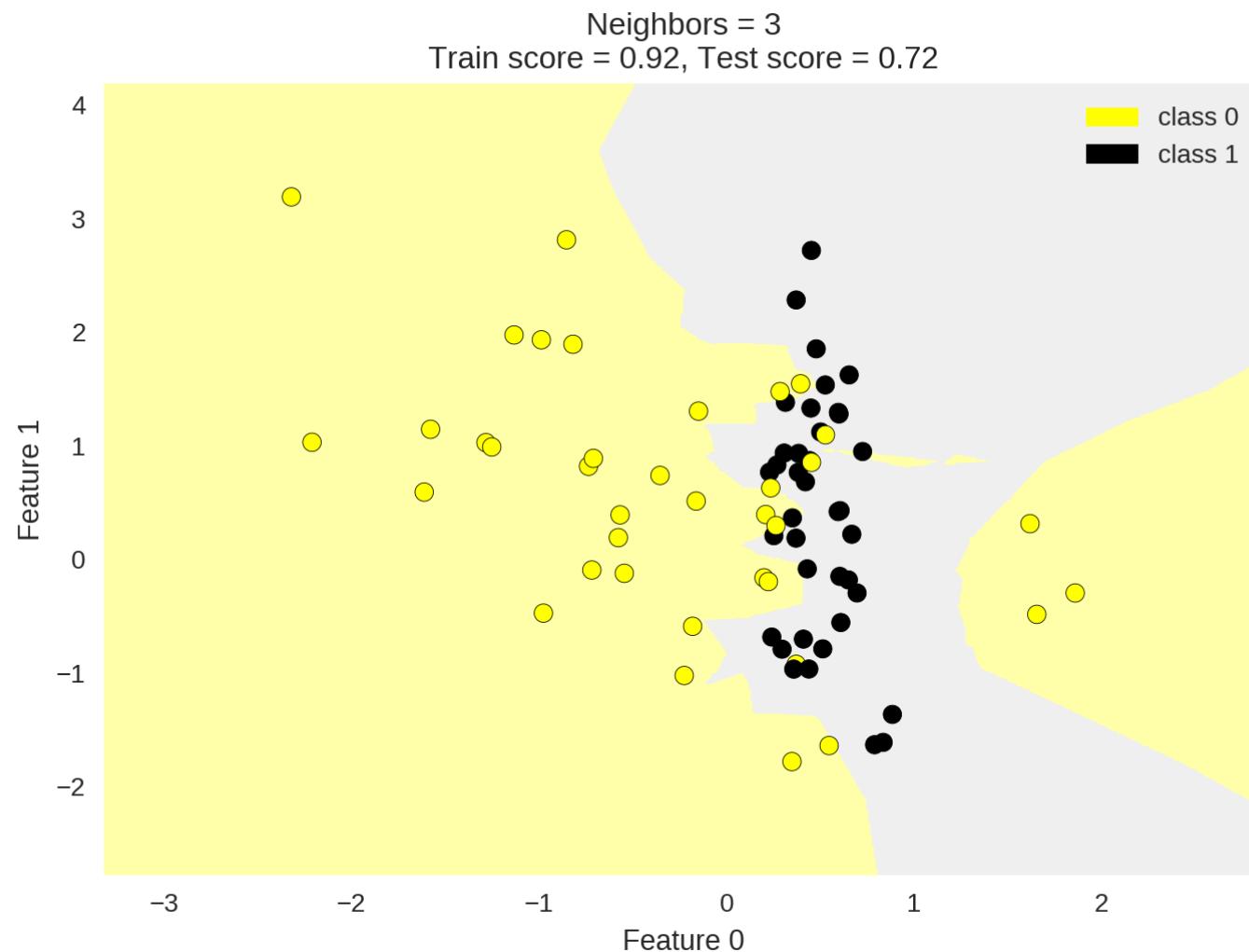
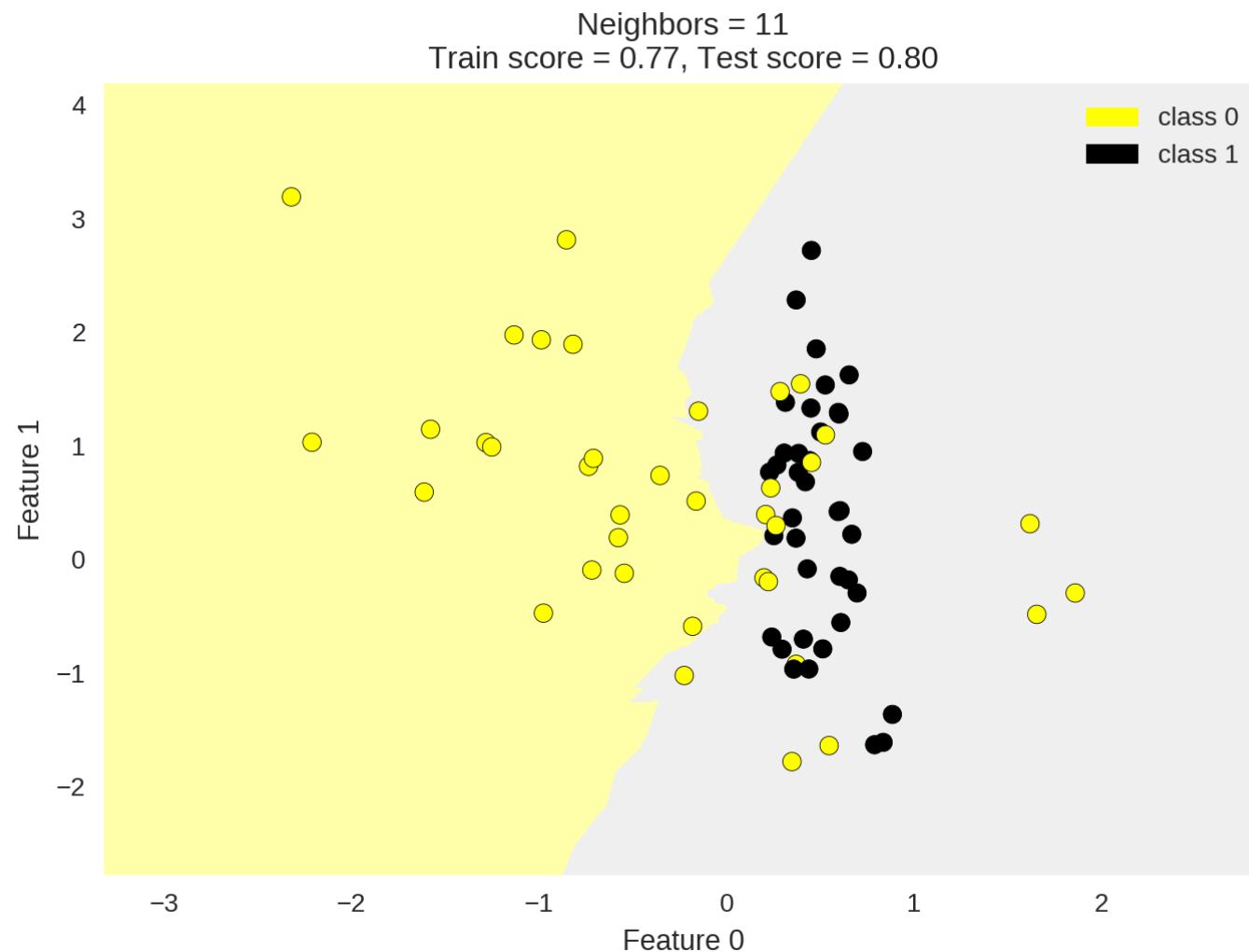
Figure 6

Figure 7

Regression

```
In [4]: from sklearn.neighbors import KNeighborsRegressor

X_train, X_test, y_train, y_test = train_test_split(X_R1, y_R1, random_state = 0)

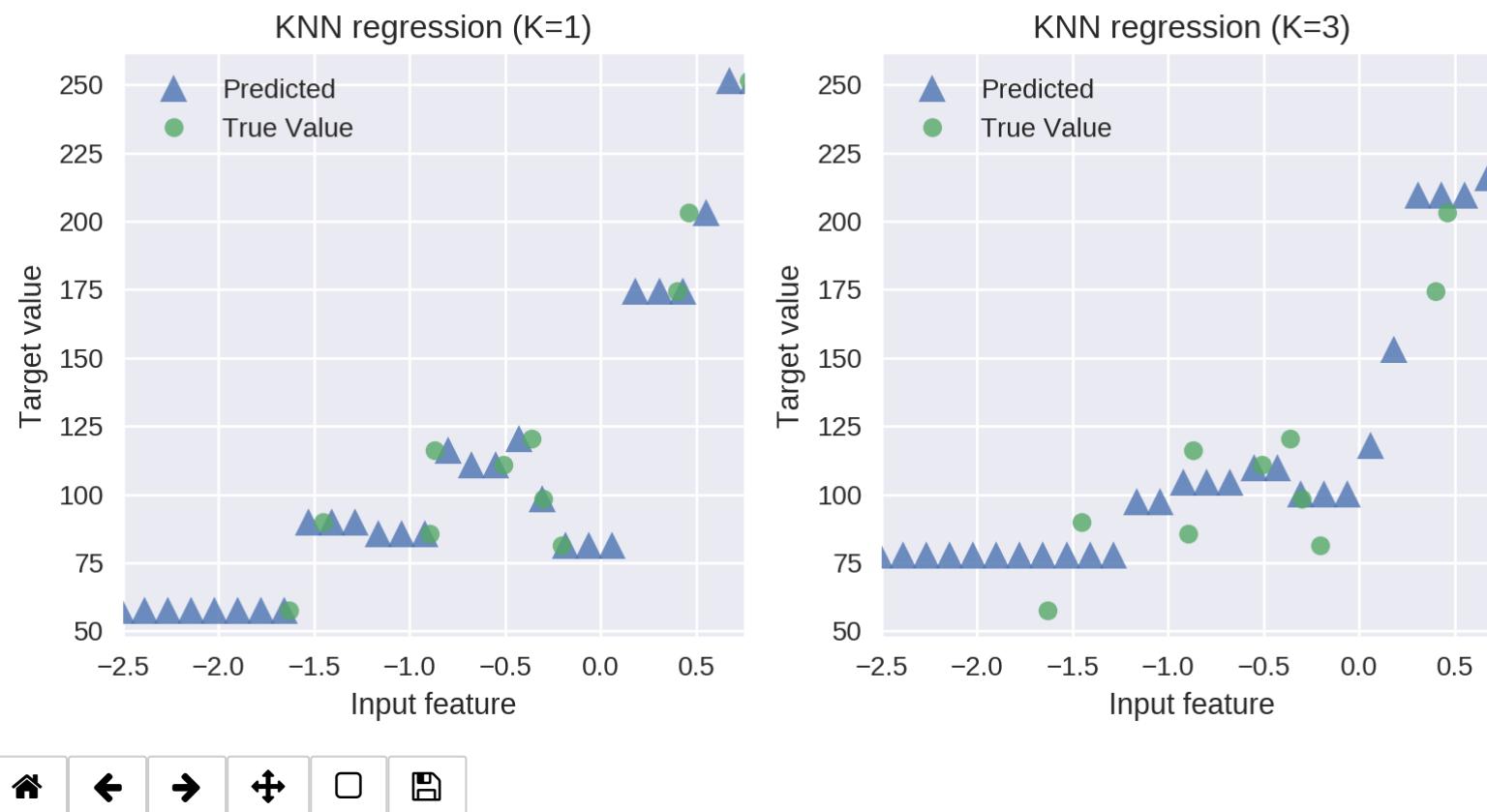
knnreg = KNeighborsRegressor(n_neighbors = 5).fit(X_train, y_train)

print(knnreg.predict(X_test))
print('R-squared test score: {:.3f}'
     .format(knnreg.score(X_test, y_test)))

[ 231.71  148.36  150.59  150.59   72.15  166.51  141.91  235.57  208.26
 102.1   191.32  134.5   228.32  148.36  159.17  113.47  144.04  199.23
 143.19  166.51  231.71  208.26  128.02  123.14  141.91]
R-squared test score: 0.425
```

```
In [5]: fig, subaxes = plt.subplots(1, 2, figsize=(8,4))
X_predict_input = np.linspace(-3, 3, 50).reshape(-1,1)
X_train, X_test, y_train, y_test = train_test_split(X_R1[0::5], y_R1[0::5], random_state = 0)

for thisaxis, K in zip(subaxes, [1, 3]):
    knnreg = KNeighborsRegressor(n_neighbors = K).fit(X_train, y_train)
    y_predict_output = knnreg.predict(X_predict_input)
    thisaxis.set_xlim([-2.5, 0.75])
    thisaxis.plot(X_predict_input, y_predict_output, '^', markersize = 10,
                  label='Predicted', alpha=0.8)
    thisaxis.plot(X_train, y_train, 'o', label='True Value', alpha=0.8)
    thisaxis.set_xlabel('Input feature')
    thisaxis.set_ylabel('Target value')
    thisaxis.set_title('KNN regression (K={})'.format(K))
    thisaxis.legend()
plt.tight_layout()
```

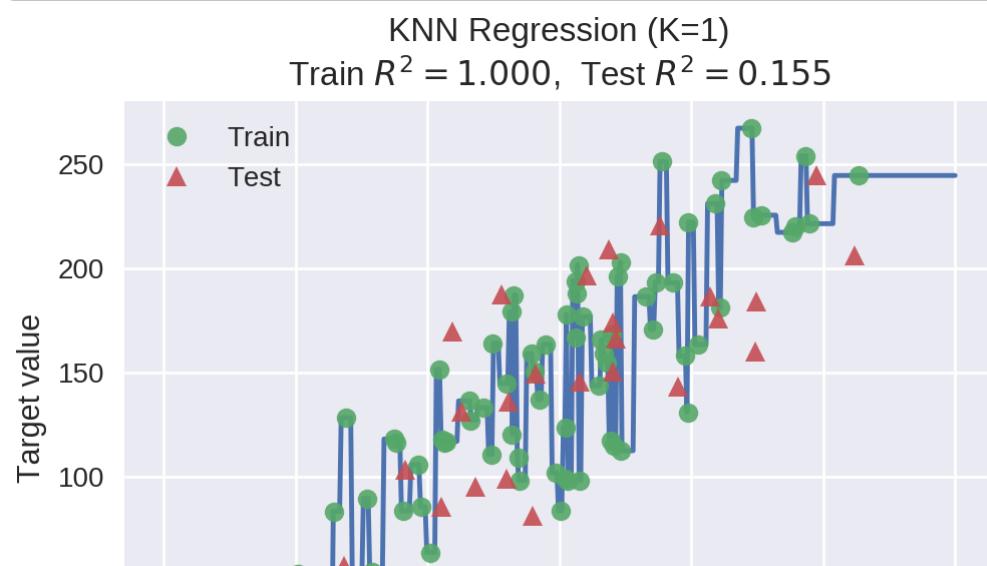
Figure 8

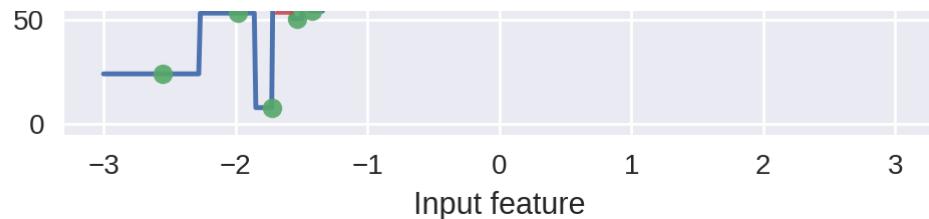
Regression model complexity as a function of K

```
In [6]: # plot k-NN regression on sample dataset for different values of K
fig, subaxes = plt.subplots(5, 1, figsize=(5,20))
X_predict_input = np.linspace(-3, 3, 500).reshape(-1,1)
X_train, X_test, y_train, y_test = train_test_split(X_R1, y_R1,
                                                    random_state = 0)

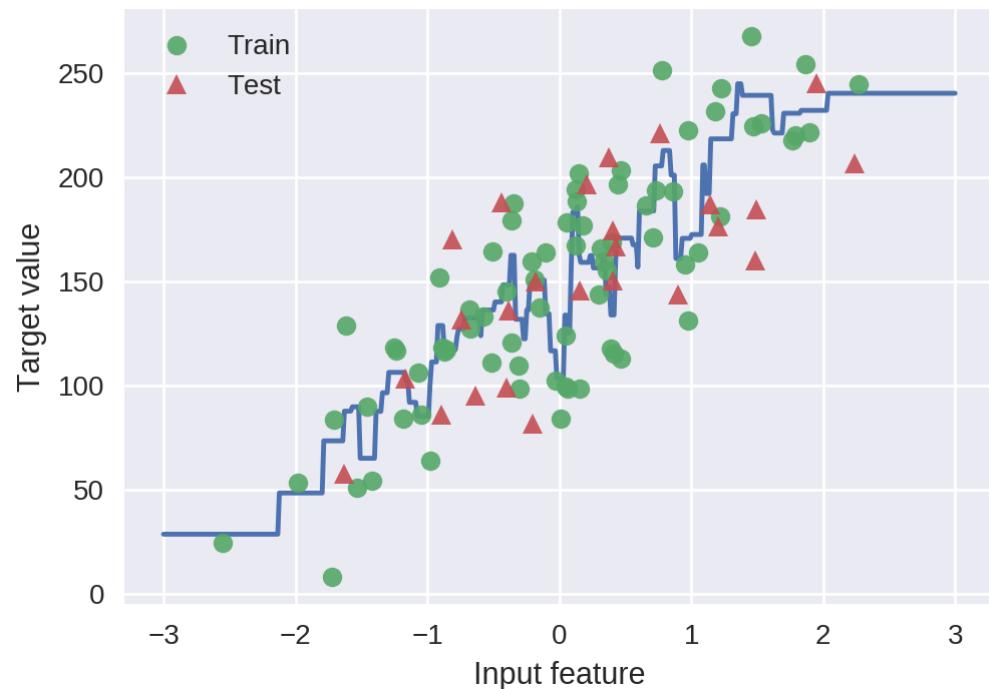
for thisaxis, K in zip(subaxes, [1, 3, 7, 15, 55]):
    knnreg = KNeighborsRegressor(n_neighbors = K).fit(X_train, y_train)
    y_predict_output = knnreg.predict(X_predict_input)
    train_score = knnreg.score(X_train, y_train)
    test_score = knnreg.score(X_test, y_test)
    thisaxis.plot(X_predict_input, y_predict_output)
    thisaxis.plot(X_train, y_train, 'o', alpha=0.9, label='Train')
    thisaxis.plot(X_test, y_test, '^', alpha=0.9, label='Test')
    thisaxis.set_xlabel('Input feature')
    thisaxis.set_ylabel('Target value')
    thisaxis.set_title('KNN Regression (K={})\n'.format(K))
    Train $R^2 = {:.3f}$, Test $R^2 = {:.3f}$'.format(K, train_score, test_score))
    thisaxis.legend()
plt.tight_layout(pad=0.4, w_pad=0.5, h_pad=1.0)
```

Figure 9



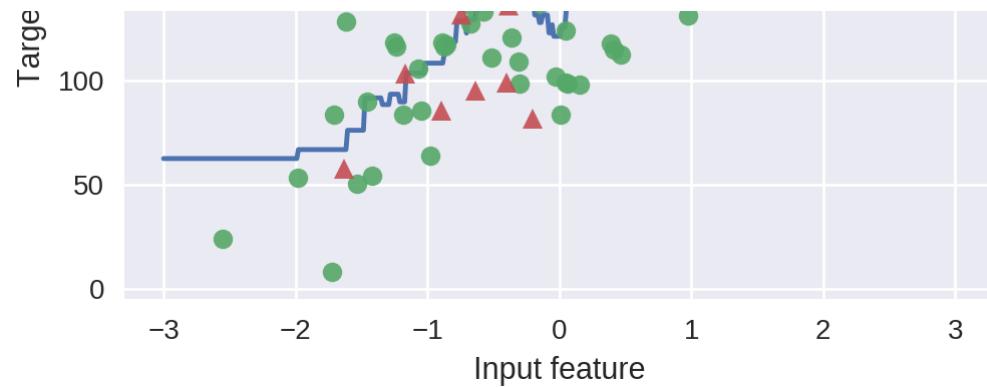


KNN Regression (K=3)
Train $R^2 = 0.797$, Test $R^2 = 0.323$

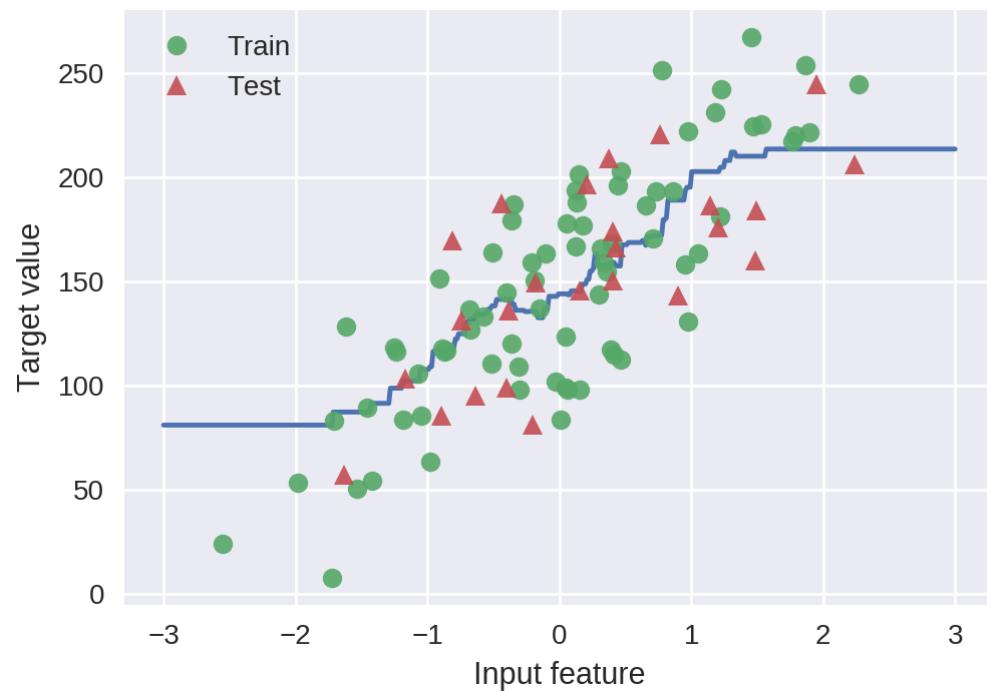


KNN Regression (K=7)
Train $R^2 = 0.720$, Test $R^2 = 0.471$

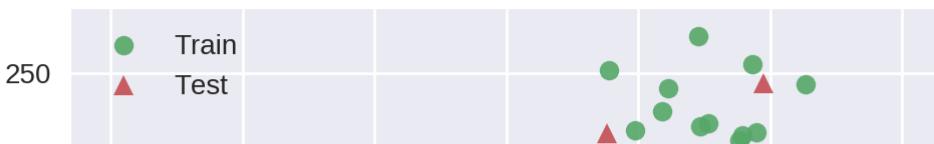


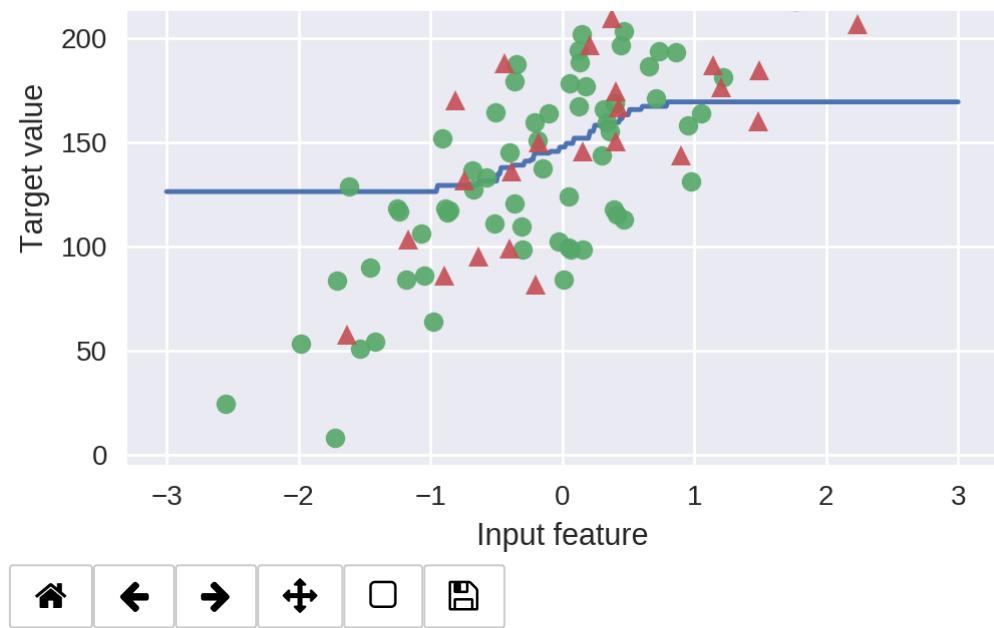


KNN Regression (K=15)
Train $R^2 = 0.647$, Test $R^2 = 0.485$



KNN Regression (K=55)
Train $R^2 = 0.357$, Test $R^2 = 0.371$





Linear models for regression

Linear regression

```
In [7]: from sklearn.linear_model import LinearRegression

X_train, X_test, y_train, y_test = train_test_split(X_R1, y_R1,
                                                    random_state = 0)
linreg = LinearRegression().fit(X_train, y_train)

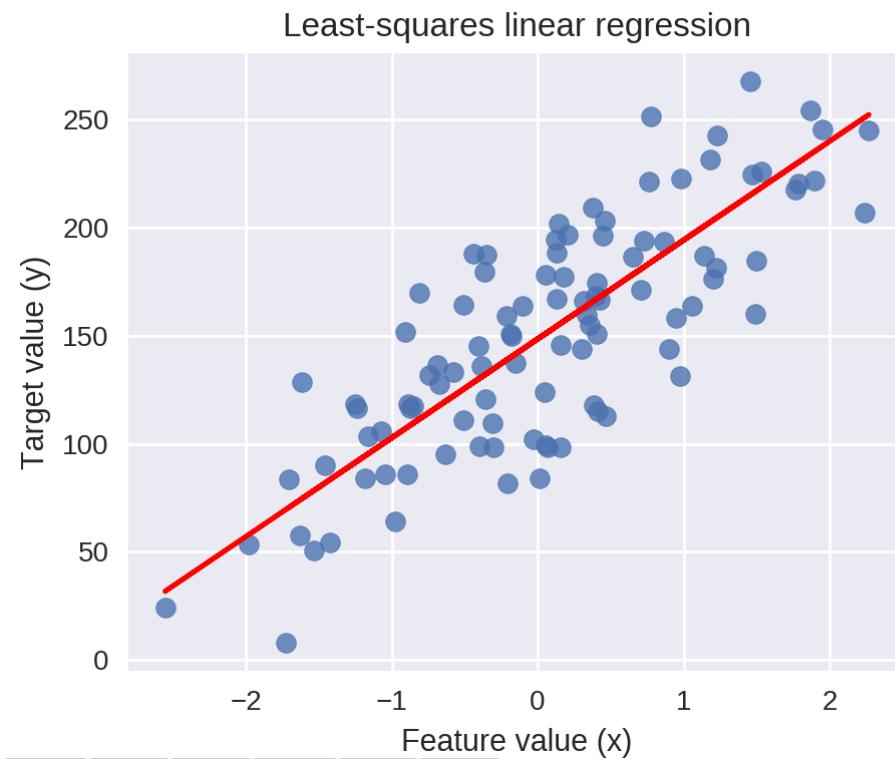
print('linear model coeff (w): {}'.format(linreg.coef_))
print('linear model intercept (b): {:.3f}'.format(linreg.intercept_))
print('R-squared score (training): {:.3f}'.format(linreg.score(X_train, y_train)))
print('R-squared score (test): {:.3f}'.format(linreg.score(X_test, y_test)))

linear model coeff (w): [ 45.71]
linear model intercept (b): 148.446
R-squared score (training): 0.679
R-squared score (test): 0.492
```

Linear regression: example plot

```
In [8]: plt.figure(figsize=(5,4))
plt.scatter(X_R1, y_R1, marker= 'o', s=50, alpha=0.8)
plt.plot(X_R1, linreg.coef_ * X_R1 + linreg.intercept_, 'r-')
plt.title('Least-squares linear regression')
plt.xlabel('Feature value (x)')
plt.ylabel('Target value (y)')
plt.show()
```

Figure 10



```
In [9]: X_train, X_test, y_train, y_test = train_test_split(X_crime, y_crime,
                                                       random_state = 0)
linreg = LinearRegression().fit(X_train, y_train)

print('Crime dataset')
print('linear model intercept: {}'
      .format(linreg.intercept_))
print('linear model coeff:\n{}'
      .format(linreg.coef_))
print('R-squared score (training): {:.3f}'
      .format(linreg.score(X_train, y_train)))
print('R-squared score (test): {:.3f}'
      .format(linreg.score(X_test, y_test)))
```

```
Crime dataset
linear model intercept: 3861.708902399444
linear model coeff:
[  1.62e-03 -1.03e+02   1.61e+01  -2.94e+01  -1.92e+00  -1.47e+01
 -2.41e-03   1.46e+00  -1.46e-02  -1.08e+01   4.35e+01  -6.92e+00
  4.95e+00  -4.11e+00  -3.63e+00   8.98e-03   8.33e-03   4.84e-03
 -5.25e+00  -1.59e+01   7.47e+00   2.31e+00  -2.48e-01   1.22e+01
 -2.90e+00  -1.49e+00   4.96e+00   5.21e+00   1.82e+02   1.15e+01
  1.54e+02  -3.40e+02  -1.22e+02   2.75e+00  -2.87e+01   2.39e+00
  9.44e-01   3.18e+00  -1.17e+01  -5.46e-03   4.24e+01  -1.10e-03
 -9.23e-01   5.13e+00  -4.69e+00   1.13e+00  -1.70e+01  -5.00e+01
  5.64e+01  -2.94e+01   3.42e-01  -3.10e+01   2.89e+01  -5.46e+01
  6.75e+02   8.54e+01  -3.35e+02  -3.17e+01   2.96e+01   7.07e+00
  7.46e+01   2.01e-02  -3.96e-01   3.15e+01   1.00e+01  -1.60e+00
 -5.63e-01   2.82e+00  -2.96e+01   1.08e+11  -1.01e-03  -1.08e+11
  1.08e+11  -3.13e+08  -4.95e-01   3.13e+08  -3.13e+08   1.47e+00
 -2.78e+00   1.12e+00  -3.70e+01   1.09e-01   3.07e-01   2.06e+01
  9.24e-01  -6.05e-01  -1.92e+00   5.88e-01]
```

R-squared score (training): 0.668
R-squared score (test): 0.520

Ridge regression

```
In [10]: from sklearn.linear_model import Ridge
X_train, X_test, y_train, y_test = train_test_split(X_crime, y_crime,
                                                    random_state = 0)

linridge = Ridge(alpha=20.0).fit(X_train, y_train)

print('Crime dataset')
print('ridge regression linear model intercept: {}'
      .format(linridge.intercept_))
print('ridge regression linear model coeff:\n{}'
      .format(linridge.coef_))
print('R-squared score (training): {:.3f}'
      .format(linridge.score(X_train, y_train)))
print('R-squared score (test): {:.3f}'
      .format(linridge.score(X_test, y_test)))
print('Number of non-zero features: {}'
      .format(np.sum(linridge.coef_ != 0)))
```

```
Crime dataset
ridge regression linear model intercept: -3352.4230358464793
ridge regression linear model coeff:
[  1.95e-03   2.19e+01   9.56e+00  -3.59e+01   6.36e+00  -1.97e+01
 -2.81e-03   1.66e+00  -6.61e-03  -6.95e+00   1.72e+01  -5.63e+00
  8.84e+00   6.79e-01  -7.34e+00   6.70e-03   9.79e-04   5.01e-03
 -4.90e+00  -1.79e+01   9.18e+00  -1.24e+00   1.22e+00   1.03e+01
 -3.78e+00  -3.73e+00   4.75e+00   8.43e+00   3.09e+01   1.19e+01
 -2.05e+00  -3.82e+01   1.85e+01   1.53e+00  -2.20e+01   2.46e+00
  3.29e-01   4.02e+00  -1.13e+01  -4.70e-03   4.27e+01  -1.23e-03
  1.41e+00   9.35e-01  -3.00e+00   1.12e+00  -1.82e+01  -1.55e+01
  2.42e+01  -1.32e+01  -4.20e-01  -3.60e+01   1.30e+01  -2.81e+01
  4.39e+01   3.87e+01  -6.46e+01  -1.64e+01   2.90e+01   4.15e+00
  5.34e+01   1.99e-02  -5.47e-01   1.24e+01   1.04e+01  -1.57e+00
  3.16e+00   8.78e+00  -2.95e+01  -2.34e-04   3.14e-04  -4.13e-04
 -1.80e-04  -5.74e-01  -5.18e-01  -4.21e-01   1.53e-01   1.33e+00
  3.85e+00   3.03e+00  -3.78e+01   1.38e-01   3.08e-01   1.57e+01
  3.31e-01   3.36e+00   1.61e-01  -2.68e+00]
```

R-squared score (training): 0.671
R-squared score (test): 0.494
Number of non-zero features: 88

Ridge regression with feature normalization

```
In [11]: from sklearn.preprocessing import MinMaxScaler
scaler = MinMaxScaler()

from sklearn.linear_model import Ridge
X_train, X_test, y_train, y_test = train_test_split(X_crime, y_crime,
                                                    random_state = 0)

X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)

linridge = Ridge(alpha=20.0).fit(X_train_scaled, y_train)

print('Crime dataset')
print('ridge regression linear model intercept: {}'
      .format(linridge.intercept_))
print('ridge regression linear model coeff:\n{}'
      .format(linridge.coef_))
print('R-squared score (training): {:.3f}'
      .format(linridge.score(X_train_scaled, y_train)))
print('R-squared score (test): {:.3f}'
      .format(linridge.score(X_test_scaled, y_test)))
print('Number of non-zero features: {}'
      .format(np.sum(linridge.coef_ != 0)))
```

```
Crime dataset
ridge regression linear model intercept: 933.3906385044113
ridge regression linear model coeff:
[ 88.69   16.49   -50.3   -82.91   -65.9    -2.28    87.74   150.95   18.88
 -31.06  -43.14  -189.44   -4.53   107.98   -76.53    2.86    34.95   90.14
  52.46  -62.11   115.02    2.67    6.94   -5.67  -101.55   -36.91   -8.71
  29.12  171.26   99.37   75.07   123.64   95.24  -330.61  -442.3  -284.5
 -258.37   17.66  -101.71   110.65   523.14   24.82    4.87   -30.47   -3.52
  50.58   10.85   18.28   44.11   58.34   67.09   -57.94   116.14   53.81
  49.02   -7.62   55.14  -52.09   123.39   77.13    45.5   184.91  -91.36
   1.08   234.09   10.39   94.72   167.92  -25.14   -1.18    14.6   36.77
   53.2   -78.86   -5.9   26.05   115.15   68.74   68.29   16.53  -97.91
  205.2    75.97   61.38  -79.83   67.27   95.67  -11.88]
```

```
R-squared score (training): 0.615
```

```
R-squared score (test): 0.599
```

```
Number of non-zero features: 88
```

Ridge regression with regularization parameter: alpha

```
In [12]: print('Ridge regression: effect of alpha regularization parameter\n')  
for this_alpha in [0, 1, 10, 20, 50, 100, 1000]:  
    linridge = Ridge(alpha = this_alpha).fit(X_train_scaled, y_train)  
    r2_train = linridge.score(X_train_scaled, y_train)  
    r2_test = linridge.score(X_test_scaled, y_test)  
    num_coeff_bigger = np.sum(abs(linridge.coef_) > 1.0)  
    print('Alpha = {:.2f}\nnum abs(coef) > 1.0: {}, '\n'r-squared training: {:.2f}, r-squared test: {:.2f}\n'.format(this_alpha, num_coeff_bigger, r2_train, r2_test))
```

Ridge regression: effect of alpha regularization parameter

```
Alpha = 0.00  
num abs(coef) > 1.0: 87, r-squared training: 0.67, r-squared test: 0.50
```

```
Alpha = 1.00  
num abs(coef) > 1.0: 87, r-squared training: 0.66, r-squared test: 0.56
```

```
Alpha = 10.00  
num abs(coef) > 1.0: 87, r-squared training: 0.63, r-squared test: 0.59
```

```
Alpha = 20.00  
num abs(coef) > 1.0: 88, r-squared training: 0.61, r-squared test: 0.60
```

```
Alpha = 50.00  
num abs(coef) > 1.0: 86, r-squared training: 0.58, r-squared test: 0.58
```

```
Alpha = 100.00  
num abs(coef) > 1.0: 87, r-squared training: 0.55, r-squared test: 0.55
```

```
Alpha = 1000.00  
num abs(coef) > 1.0: 84, r-squared training: 0.31, r-squared test: 0.30
```

Lasso regression

```
In [13]: from sklearn.linear_model import Lasso
from sklearn.preprocessing import MinMaxScaler
scaler = MinMaxScaler()

X_train, X_test, y_train, y_test = train_test_split(X_crime, y_crime,
                                                    random_state = 0)

X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)

linlasso = Lasso(alpha=2.0, max_iter = 10000).fit(X_train_scaled, y_train)

print('Crime dataset')
print('lasso regression linear model intercept: {}'
      .format(linlasso.intercept_))
print('lasso regression linear model coeff:\n{}'
      .format(linlasso.coef_))
print('Non-zero features: {}'
      .format(np.sum(linlasso.coef_ != 0)))
print('R-squared score (training): {:.3f}'
      .format(linlasso.score(X_train_scaled, y_train)))
print('R-squared score (test): {:.3f}\n'
      .format(linlasso.score(X_test_scaled, y_test)))
print('Features with non-zero weight (sorted by absolute magnitude):')

for e in sorted (list(zip(list(X_crime), linlasso.coef_)),
                 key = lambda e: -abs(e[1])):
    if e[1] != 0:
        print('\t{}, {:.3f}'.format(e[0], e[1]))
```

```
Crime dataset
lasso regression linear model intercept: 1186.6120619985809
lasso regression linear model coeff:
[ 0.          0.          -0.         -168.18     -0.          -0.          0.           119.69
  0.          -0.          0.         -169.68     -0.          0.          -0.          0.
  0.          0.          -0.         -0.          0.          -0.          0.          0.
 -57.53       -0.          -0.          0.          259.33     -0.          0.          0.
  0.          -0.         -1188.74    -0.          -0.          -0.         -231.42    0.
 1488.37      0.          -0.         -0.          -0.          0.          0.          0.
  0.          0.          -0.          0.          20.14      0.          0.          0.
  0.          0.          339.04     0.          0.          459.54     -0.          0.
```

122.69	-0.	91.41	0.	-0.	0.	0.	73.14
0.	-0.	0.	0.	86.36	0.	0.	0.
-104.57	264.93	0.	23.45	-49.39	0.	5.2	0.]

Non-zero features: 20

R-squared score (training): 0.631

R-squared score (test): 0.624

Features with non-zero weight (sorted by absolute magnitude):

- PctKidsBornNeverMar, 1488.365
- PctKids2Par, -1188.740
- HousVacant, 459.538
- PctPersDenseHous, 339.045
- NumInShelters, 264.932
- MalePctDivorce, 259.329
- PctWorkMom, -231.423
- pctWInvInc, -169.676
- agePct12t29, -168.183
- PctVacantBoarded, 122.692
- pctUrban, 119.694
- MedOwnCostPctIncNoMtg, -104.571
- MedYrHousBuilt, 91.412
- RentOrange, 86.356
- OwnOccHiQuart, 73.144
- PctEmplManu, -57.530
- PctBornSameState, -49.394
- PctForeignBorn, 23.449
- PctLargHouseFam, 20.144
- PctSameCity85, 5.198

Lasso regression with regularization parameter: alpha

```
In [14]: print('Lasso regression: effect of alpha regularization\n\\
parameter on number of features kept in final model\\n')

for alpha in [0.5, 1, 2, 3, 5, 10, 20, 50]:
    linlasso = Lasso(alpha, max_iter = 10000).fit(X_train_scaled, y_train)
    r2_train = linlasso.score(X_train_scaled, y_train)
    r2_test = linlasso.score(X_test_scaled, y_test)

    print('Alpha = {:.2f}\\nFeatures kept: {}, r-squared training: {:.2f}, \
r-squared test: {:.2f}\\n'
          .format(alpha, np.sum(linlasso.coef_ != 0), r2_train, r2_test))
```

Lasso regression: effect of alpha regularization
parameter on number of features kept in final model

Alpha = 0.50

Features kept: 35, r-squared training: 0.65, r-squared test: 0.58

Alpha = 1.00

Features kept: 25, r-squared training: 0.64, r-squared test: 0.60

Alpha = 2.00

Features kept: 20, r-squared training: 0.63, r-squared test: 0.62

Alpha = 3.00

Features kept: 17, r-squared training: 0.62, r-squared test: 0.63

Alpha = 5.00

Features kept: 12, r-squared training: 0.60, r-squared test: 0.61

Alpha = 10.00

Features kept: 6, r-squared training: 0.57, r-squared test: 0.58

Alpha = 20.00

Features kept: 2, r-squared training: 0.51, r-squared test: 0.50

Alpha = 50.00

Features kept: 1, r-squared training: 0.31, r-squared test: 0.30

Polynomial regression

```
In [15]: from sklearn.linear_model import LinearRegression
from sklearn.linear_model import Ridge
from sklearn.preprocessing import PolynomialFeatures

X_train, X_test, y_train, y_test = train_test_split(X_F1, y_F1,
                                                    random_state = 0)
linreg = LinearRegression().fit(X_train, y_train)

print('linear model coeff (w): {}'
      .format(linreg.coef_))
print('linear model intercept (b): {:.3f}'
      .format(linreg.intercept_))
print('R-squared score (training): {:.3f}'
      .format(linreg.score(X_train, y_train)))
print('R-squared score (test): {:.3f}'
      .format(linreg.score(X_test, y_test)))

print('\nNow we transform the original input data to add\n'
      'polynomial features up to degree 2 (quadratic)\n')
poly = PolynomialFeatures(degree=2)
X_F1_poly = poly.fit_transform(X_F1)

X_train, X_test, y_train, y_test = train_test_split(X_F1_poly, y_F1,
                                                    random_state = 0)
linreg = LinearRegression().fit(X_train, y_train)

print('(poly deg 2) linear model coeff (w):\n{}'
      .format(linreg.coef_))
print('(poly deg 2) linear model intercept (b): {:.3f}'
      .format(linreg.intercept_))
print('(poly deg 2) R-squared score (training): {:.3f}'
      .format(linreg.score(X_train, y_train)))
print('(poly deg 2) R-squared score (test): {:.3f}\n'
      .format(linreg.score(X_test, y_test)))

print('\nAddition of many polynomial features often leads to\n'
      'overfitting, so we often use polynomial features in combination\n'
      'with regression that has a regularization penalty, like ridge\n'
      'regression.\n')
```

```

X_train, X_test, y_train, y_test = train_test_split(X_F1_poly, y_F1,
                                                random_state = 0)
linreg = Ridge().fit(X_train, y_train)

print('(poly deg 2 + ridge) linear model coeff (w):\n{}'
      .format(linreg.coef_))
print('(poly deg 2 + ridge) linear model intercept (b): {:.3f}'
      .format(linreg.intercept_))
print('(poly deg 2 + ridge) R-squared score (training): {:.3f}'
      .format(linreg.score(X_train, y_train)))
print('(poly deg 2 + ridge) R-squared score (test): {:.3f}'
      .format(linreg.score(X_test, y_test)))

linear model coeff (w): [ 4.42   6.       0.53  10.24  6.55  -2.02  -0.32]
linear model intercept (b): 1.543
R-squared score (training): 0.722
R-squared score (test): 0.722

```

Now we transform the original input data to add polynomial features up to degree 2 (quadratic)

```

(poly deg 2) linear model coeff (w):
[ 3.41e-12  1.66e+01  2.67e+01 -2.21e+01  1.24e+01  6.93e+00
  1.05e+00  3.71e+00 -1.34e+01 -5.73e+00  1.62e+00  3.66e+00
  5.05e+00 -1.46e+00  1.95e+00 -1.51e+01  4.87e+00 -2.97e+00
 -7.78e+00  5.15e+00 -4.65e+00  1.84e+01 -2.22e+00  2.17e+00
 -1.28e+00  1.88e+00  1.53e-01  5.62e-01 -8.92e-01 -2.18e+00
  1.38e+00 -4.90e+00 -2.24e+00  1.38e+00 -5.52e-01 -1.09e+00]
(poly deg 2) linear model intercept (b): -3.206
(poly deg 2) R-squared score (training): 0.969
(poly deg 2) R-squared score (test): 0.805

```

Addition of many polynomial features often leads to overfitting, so we often use polynomial features in combination with regression that has a regularization penalty, like ridge regression.

```

(poly deg 2 + ridge) linear model coeff (w):
[ 0.     2.23  4.73 -3.15  3.86  1.61 -0.77 -0.15 -1.75  1.6    1.37  2.52
  2.72  0.49 -1.94 -1.63  1.51  0.89  0.26  2.05 -1.93  3.62 -0.72  0.63
 -3.16  1.29  3.55  1.73  0.94 -0.51  1.7   -1.98  1.81 -0.22  2.88 -0.89]

```

```
(poly deg 2 + ridge) linear model intercept (b): 5.418
(poly deg 2 + ridge) R-squared score (training): 0.826
(poly deg 2 + ridge) R-squared score (test): 0.825
```

Linear models for classification

Logistic regression

Logistic regression for binary classification on fruits dataset using height, width features (positive class: apple, negative class: others)

```
In [16]: from sklearn.linear_model import LogisticRegression
from adspy_shared_utilities import (
plot_class_regions_for_classifier_subplot)

fig, subaxes = plt.subplots(1, 1, figsize=(7, 5))
y_fruits_apple = y_fruits_2d == 1    # make into a binary problem: apples vs everything else
X_train, X_test, y_train, y_test = (
train_test_split(X_fruits_2d.as_matrix(),
                 y_fruits_apple.as_matrix(),
                 random_state = 0))

clf = LogisticRegression(C=100).fit(X_train, y_train)
plot_class_regions_for_classifier_subplot(clf, X_train, y_train, None,
                                         None, 'Logistic regression \
for binary classification\nFruit dataset: Apple vs others',
                                         subaxes)

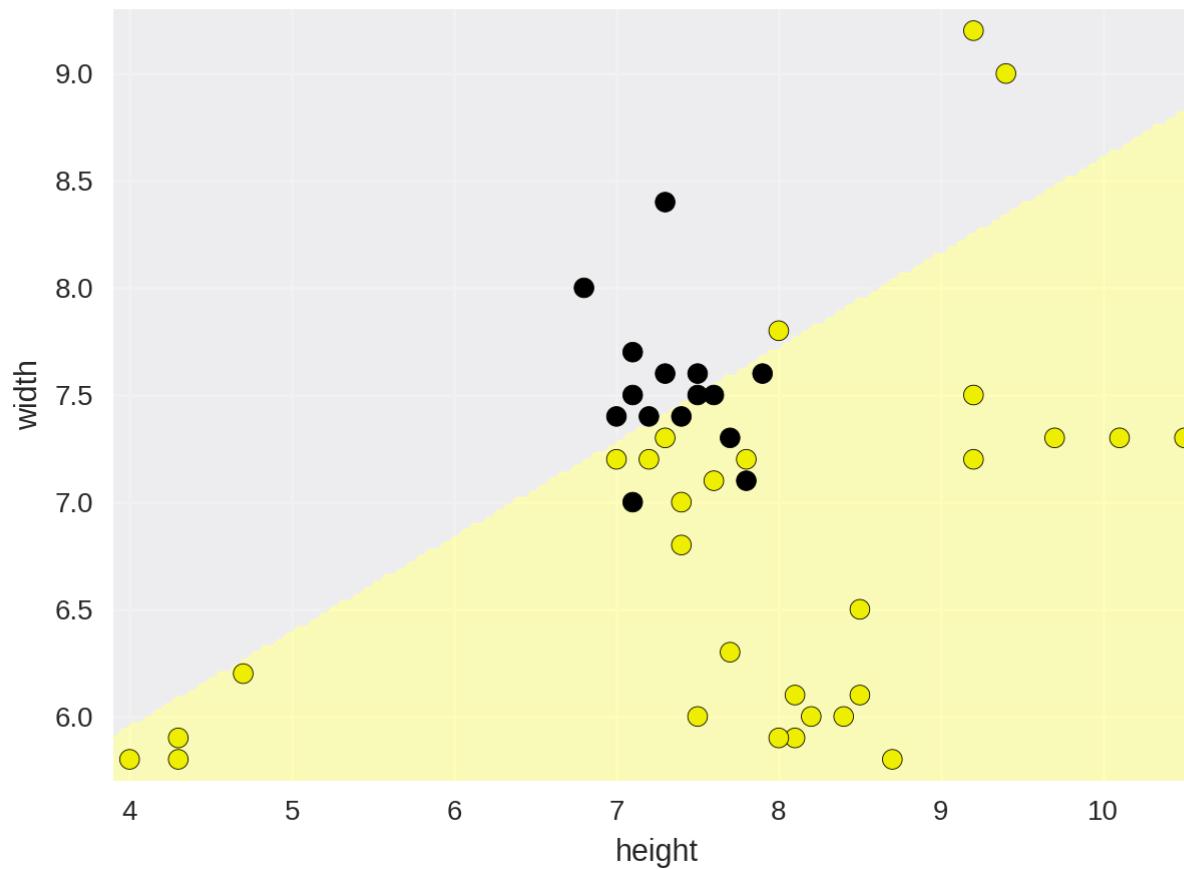
h = 6
w = 8
print('A fruit with height {} and width {} is predicted to be: {}'
      .format(h,w, ['not an apple', 'an apple'][clf.predict([[h,w]])[0]]))

h = 10
w = 7
print('A fruit with height {} and width {} is predicted to be: {}'
      .format(h,w, ['not an apple', 'an apple'][clf.predict([[h,w]])[0]]))
subaxes.set_xlabel('height')
subaxes.set_ylabel('width')

print('Accuracy of Logistic regression classifier on training set: {:.2f}'
      .format(clf.score(X_train, y_train)))
print('Accuracy of Logistic regression classifier on test set: {:.2f}'
      .format(clf.score(X_test, y_test)))
```

Figure 11

Logistic regression for binary classification
Fruit dataset: Apple vs others



A fruit with height 6 and width 8 is predicted to be: an apple
A fruit with height 10 and width 7 is predicted to be: not an apple
Accuracy of Logistic regression classifier on training set: 0.77
Accuracy of Logistic regression classifier on test set: 0.73

Logistic regression on simple synthetic dataset

```
In [17]: from sklearn.linear_model import LogisticRegression
from adspy_shared_utilities import (
plot_class_regions_for_classifier_subplot)

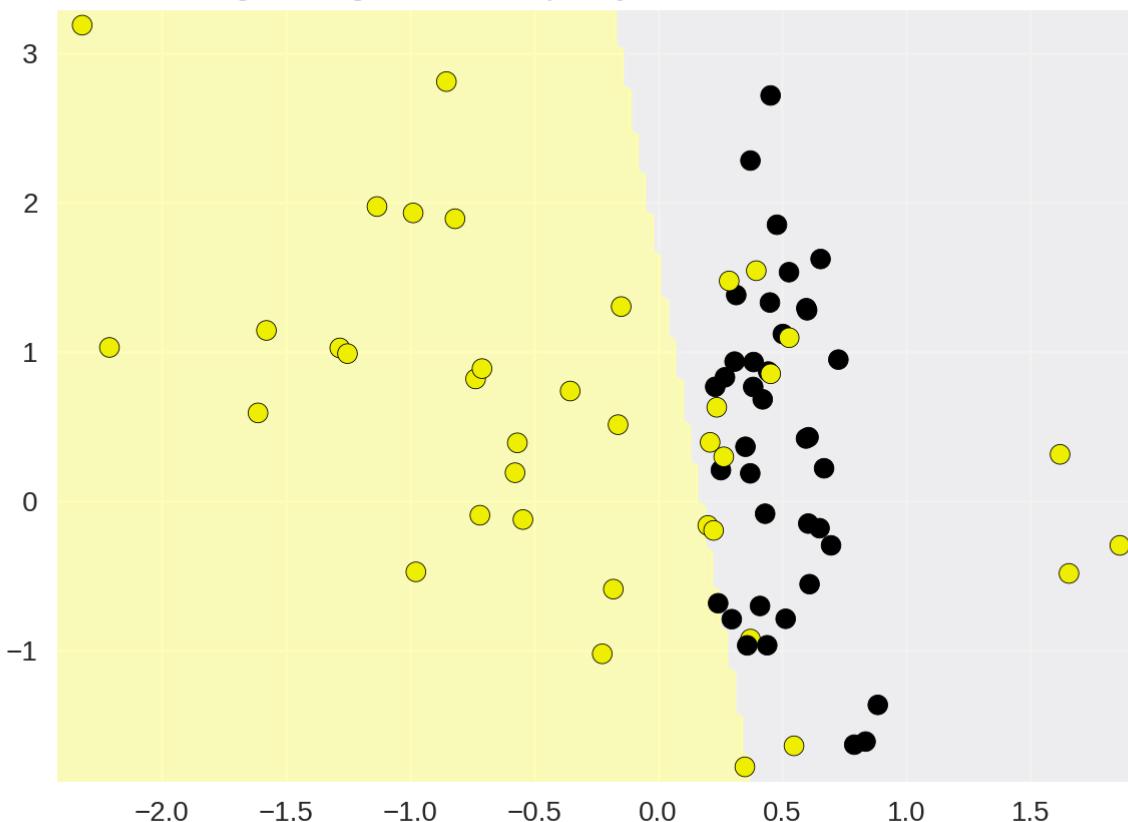
X_train, X_test, y_train, y_test = train_test_split(X_C2, y_C2,
                                                    random_state = 0)

fig, subaxes = plt.subplots(1, 1, figsize=(7, 5))
clf = LogisticRegression().fit(X_train, y_train)
title = 'Logistic regression, simple synthetic dataset C = {:.3f}'.format(1.0)
plot_class_regions_for_classifier_subplot(clf, X_train, y_train,
                                         None, None, title, subaxes)

print('Accuracy of Logistic regression classifier on training set: {:.2f}'
      .format(clf.score(X_train, y_train)))
print('Accuracy of Logistic regression classifier on test set: {:.2f}'
      .format(clf.score(X_test, y_test)))
```

Figure 12

Logistic regression, simple synthetic dataset C = 1.000



Accuracy of Logistic regression classifier on training set: 0.80
Accuracy of Logistic regression classifier on test set: 0.80

Logistic regression regularization: C parameter

```
In [18]: X_train, X_test, y_train, y_test = (
    train_test_split(X_fruits_2d.as_matrix(),
                     y_fruits_apple.as_matrix(),
                     random_state=0))

fig, subaxes = plt.subplots(3, 1, figsize=(4, 10))

for this_C, subplot in zip([0.1, 1, 100], subaxes):
    clf = LogisticRegression(C=this_C).fit(X_train, y_train)
    title = 'Logistic regression (apple vs rest), C = {:.3f}'.format(this_C)

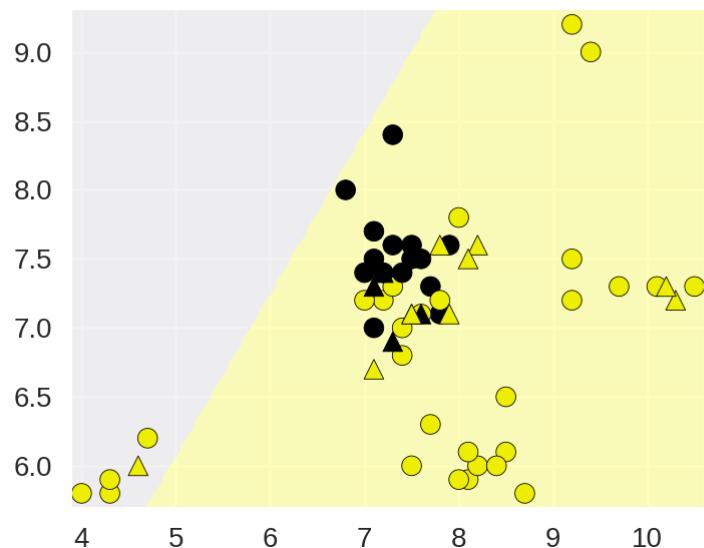
    plot_class_regions_for_classifier_subplot(clf, X_train, y_train,
                                              X_test, y_test, title,
                                              subplot)

plt.tight_layout()
```

Figure 13

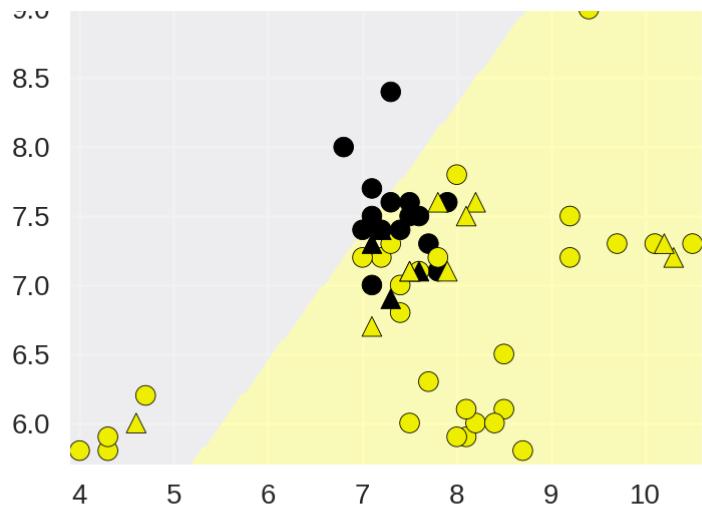


Logistic regression (apple vs rest), C = 0.100
Train score = 0.57, Test score = 0.67

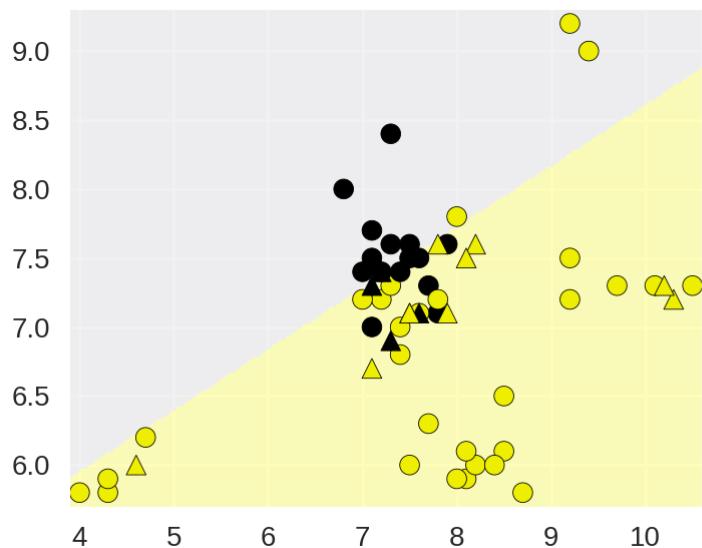


Logistic regression (apple vs rest), C = 1.000
Train score = 0.68, Test score = 0.60





Logistic regression (apple vs rest), C = 100.000
Train score = 0.77, Test score = 0.73



Application to real dataset

```
In [19]: from sklearn.linear_model import LogisticRegression

X_train, X_test, y_train, y_test = train_test_split(X_cancer, y_cancer, random_state = 0)

clf = LogisticRegression().fit(X_train, y_train)
print('Breast cancer dataset')
print('Accuracy of Logistic regression classifier on training set: {:.2f}'
      .format(clf.score(X_train, y_train)))
print('Accuracy of Logistic regression classifier on test set: {:.2f}'
      .format(clf.score(X_test, y_test)))

Breast cancer dataset
Accuracy of Logistic regression classifier on training set: 0.96
Accuracy of Logistic regression classifier on test set: 0.96
```

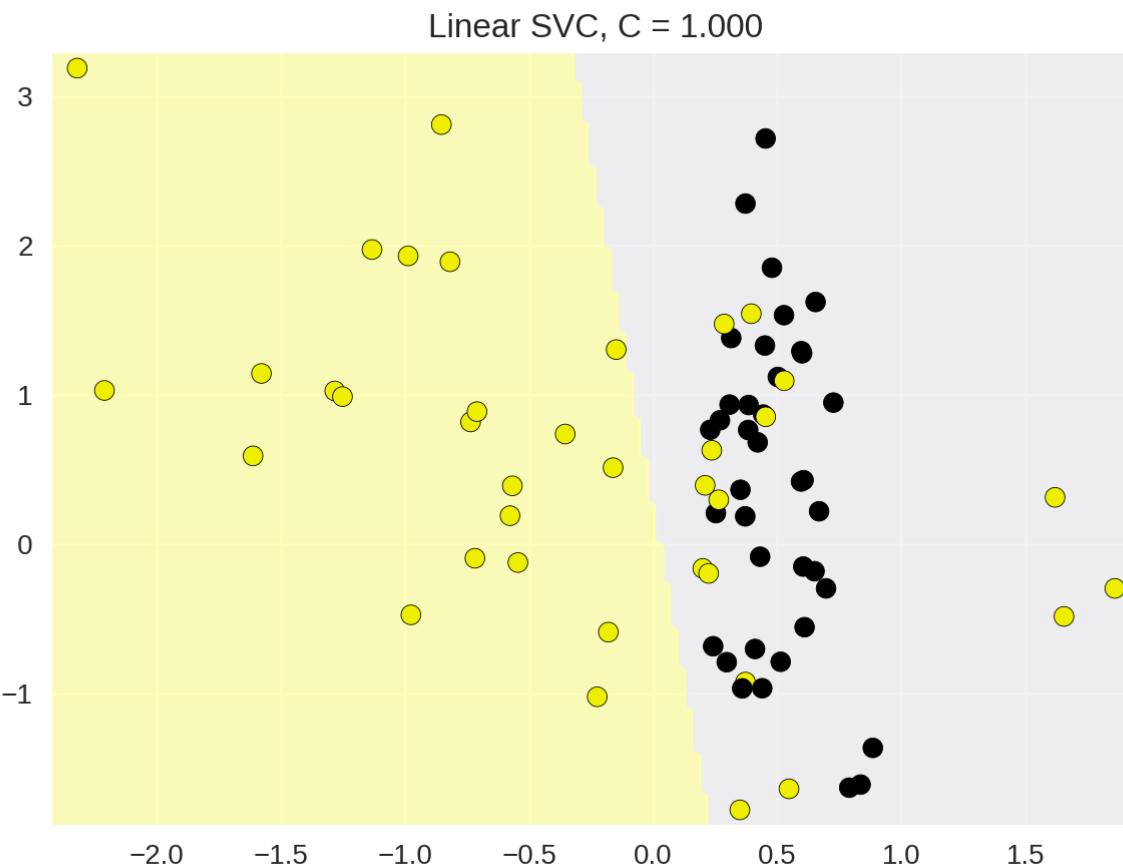
Support Vector Machines

Linear Support Vector Machine

```
In [20]: from sklearn.svm import SVC
from adspy_shared_utilities import plot_class_regions_for_classifier_subplot

X_train, X_test, y_train, y_test = train_test_split(X_C2, y_C2, random_state = 0)

fig, subaxes = plt.subplots(1, 1, figsize=(7, 5))
this_C = 1.0
clf = SVC(kernel = 'linear', C=this_C).fit(X_train, y_train)
title = 'Linear SVC, C = {:.3f}'.format(this_C)
plot_class_regions_for_classifier_subplot(clf, X_train, y_train, None, None, title, subaxes)
```

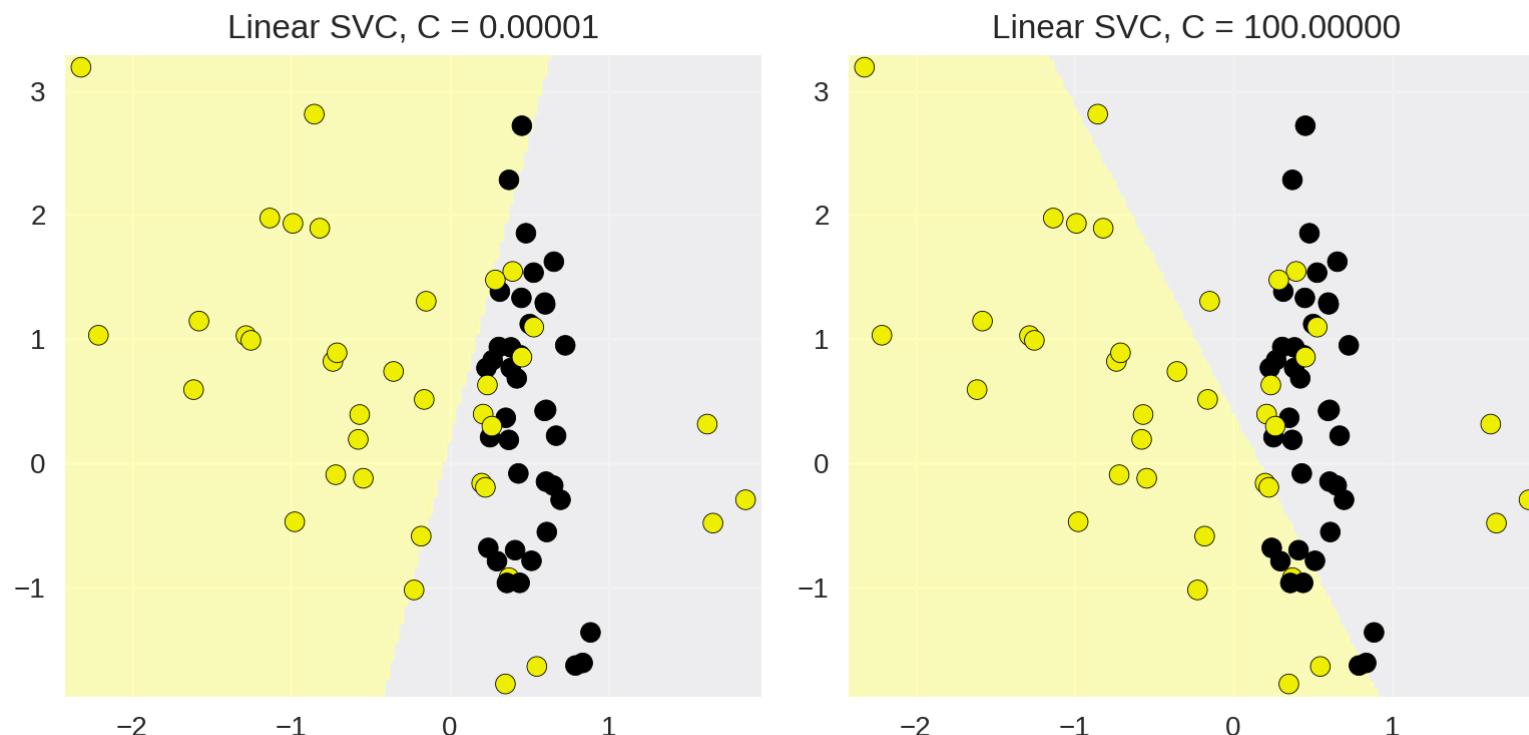
Figure 14**Linear Support Vector Machine: C parameter**

```
In [21]: from sklearn.svm import LinearSVC
from adspy_shared_utilities import plot_class_regions_for_classifier

X_train, X_test, y_train, y_test = train_test_split(X_C2, y_C2, random_state = 0)
fig, subaxes = plt.subplots(1, 2, figsize=(8, 4))

for this_C, subplot in zip([0.00001, 100], subaxes):
    clf = LinearSVC(C=this_C).fit(X_train, y_train)
    title = 'Linear SVC, C = {:.5f}'.format(this_C)
    plot_class_regions_for_classifier_subplot(clf, X_train, y_train,
                                              None, None, title, subplot)
plt.tight_layout()
```

Figure 15



Application to real dataset

```
In [22]: from sklearn.svm import LinearSVC
X_train, X_test, y_train, y_test = train_test_split(X_cancer, y_cancer, random_state = 0)

clf = LinearSVC().fit(X_train, y_train)
print('Breast cancer dataset')
print('Accuracy of Linear SVC classifier on training set: {:.2f}'
     .format(clf.score(X_train, y_train)))
print('Accuracy of Linear SVC classifier on test set: {:.2f}'
     .format(clf.score(X_test, y_test)))

Breast cancer dataset
Accuracy of Linear SVC classifier on training set: 0.90
Accuracy of Linear SVC classifier on test set: 0.90
```

Multi-class classification with linear models

LinearSVC with M classes generates M one vs rest classifiers.

```
In [23]: from sklearn.svm import LinearSVC

X_train, X_test, y_train, y_test = train_test_split(X_fruits_2d, y_fruits_2d, random_state = 0)

clf = LinearSVC(C=5, random_state = 67).fit(X_train, y_train)
print('Coefficients:\n', clf.coef_)
print('Intercepts:\n', clf.intercept_)

Coefficients:
[[-0.26  0.71]
 [-1.63  1.16]
 [ 0.03  0.29]
 [ 1.24 -1.64]]
Intercepts:
[-3.29  1.2 -2.72  1.16]
```

Multi-class results on the fruit dataset

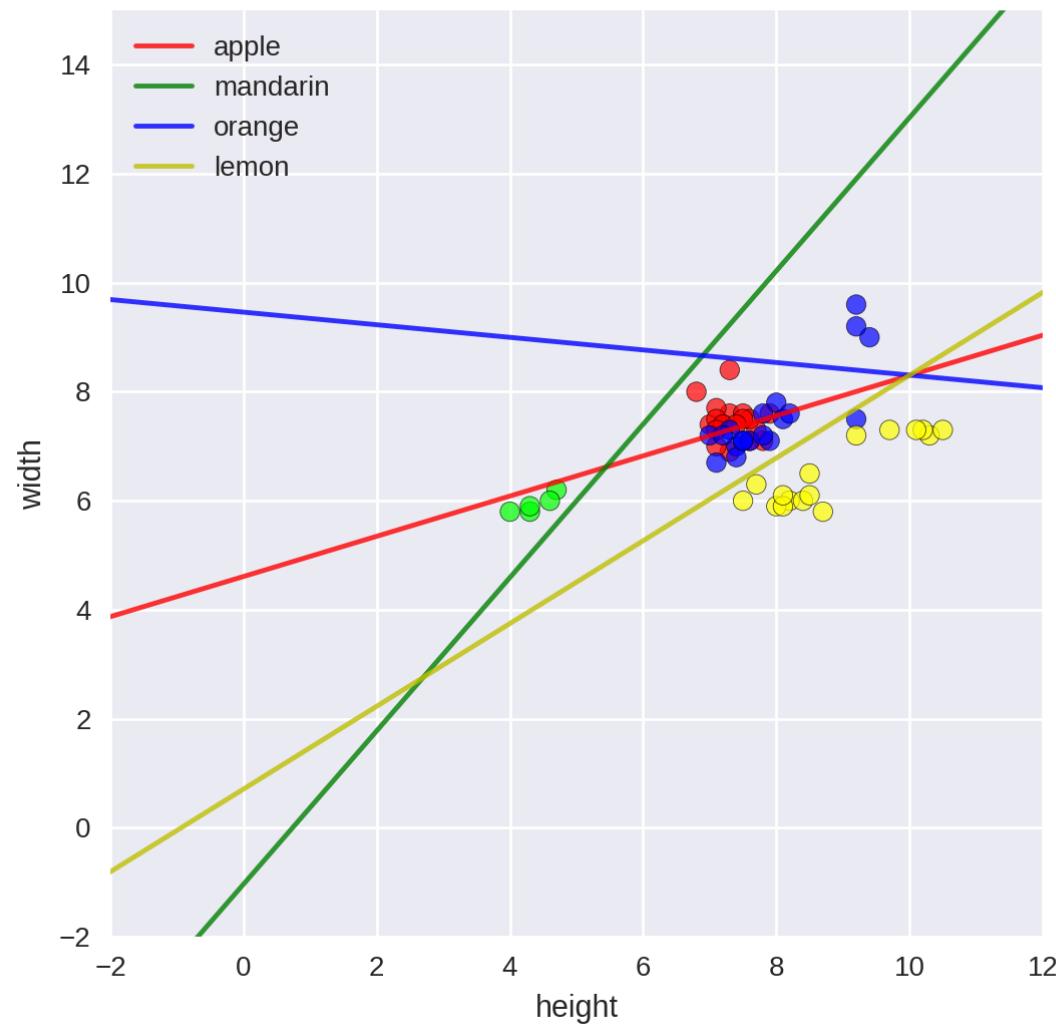

```
In [24]: plt.figure(figsize=(6,6))
colors = ['r', 'g', 'b', 'y']
cmap_fruits = ListedColormap(['#FF0000', '#00FF00', '#0000FF', '#FFFF00'])

plt.scatter(x_fruits_2d[['height']], x_fruits_2d[['width']],
            c=y_fruits_2d, cmap=cmap_fruits, edgecolor = 'black', alpha=.7)

x_0_range = np.linspace(-10, 15)

for w, b, color in zip(clf.coef_, clf.intercept_, ['r', 'g', 'b', 'y']):
    # Since class prediction with a linear model uses the formula  $y = w_0 x_0 + w_1 x_1 + b$ ,
    # and the decision boundary is defined as being all points with  $y = 0$ , to plot  $x_1$  as a
    # function of  $x_0$  we just solve  $w_0 x_0 + w_1 x_1 + b = 0$  for  $x_1$ :
    plt.plot(x_0_range, -(x_0_range * w[0] + b) / w[1], c=color, alpha=.8)

plt.legend(target_names_fruits)
plt.xlabel('height')
plt.ylabel('width')
plt.xlim(-2, 12)
plt.ylim(-2, 15)
plt.show()
```

Figure 16

Kernelized Support Vector Machines

Classification

```
In [25]: from sklearn.svm import SVC
from adspy_shared_utilities import plot_class_regions_for_classifier

X_train, X_test, y_train, y_test = train_test_split(X_D2, y_D2, random_state = 0)

# The default SVC kernel is radial basis function (RBF)
plot_class_regions_for_classifier(SVC().fit(X_train, y_train),
                                  X_train, y_train, None, None,
                                  'Support Vector Classifier: RBF kernel')

# Compare decision boundries with polynomial kernel, degree = 3
plot_class_regions_for_classifier(SVC(kernel = 'poly', degree = 3)
                                  .fit(X_train, y_train), X_train,
                                  y_train, None, None,
                                  'Support Vector Classifier: Polynomial kernel, degree = 3')
```

Figure 17

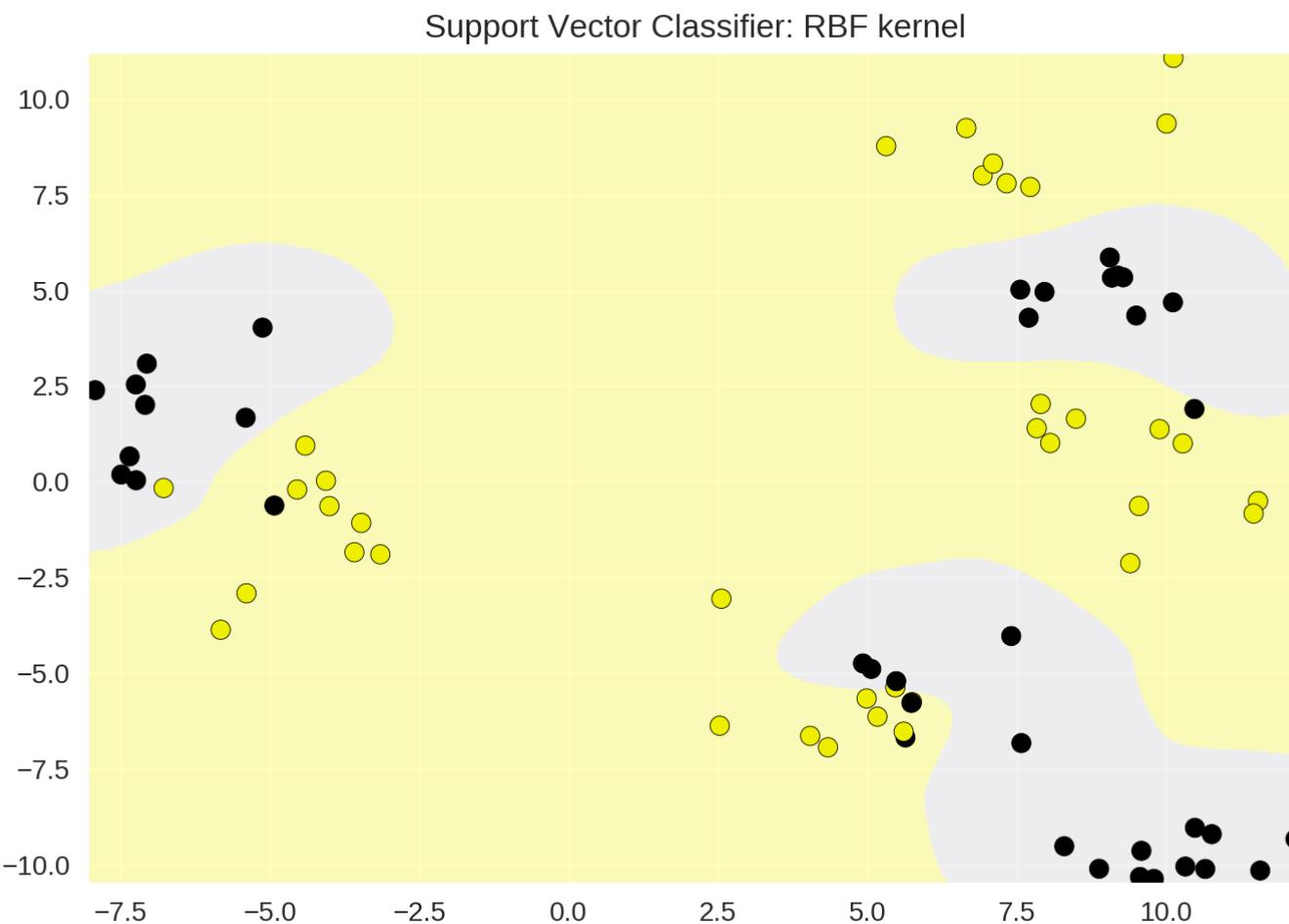
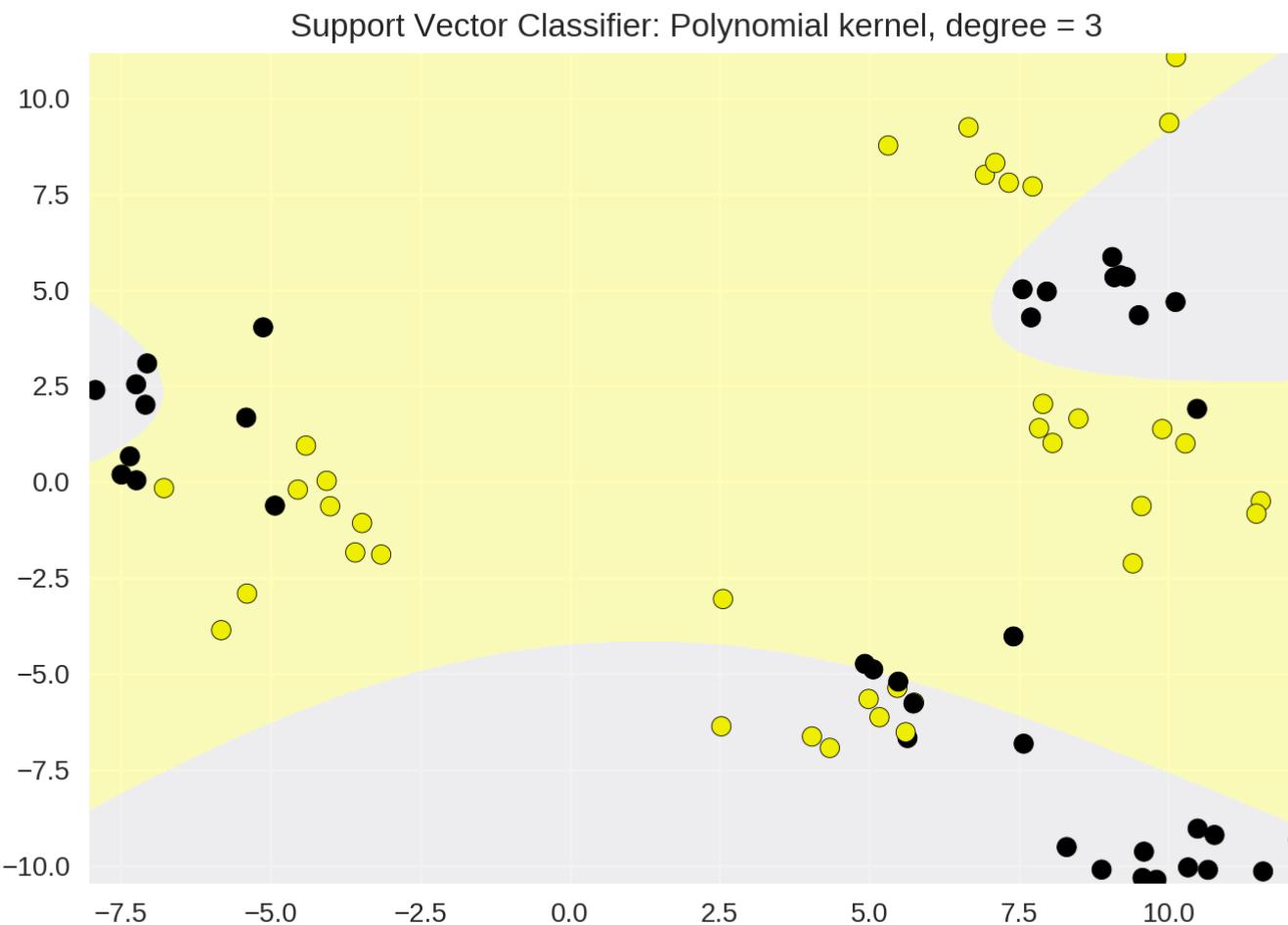


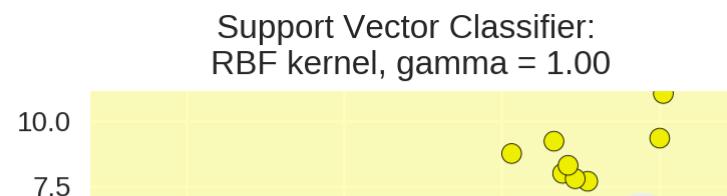
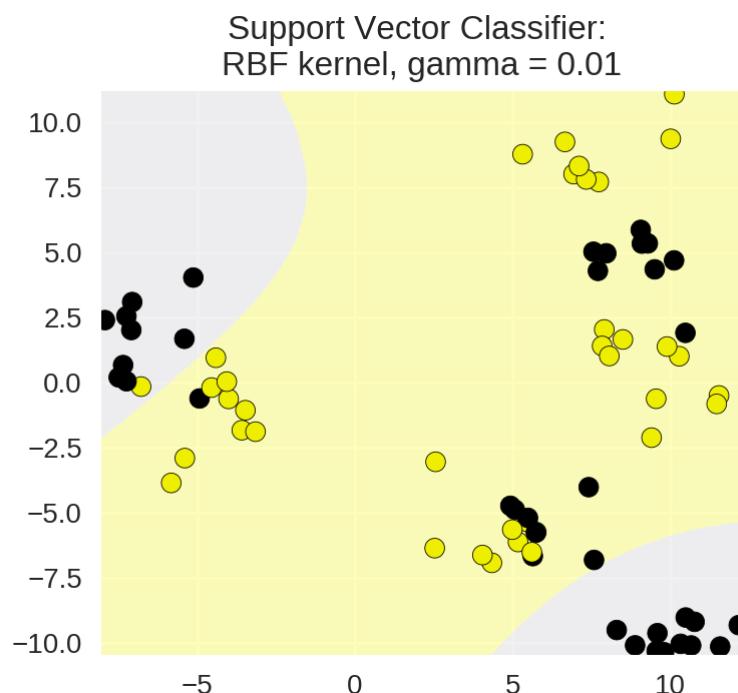
Figure 18**Support Vector Machine with RBF kernel: gamma parameter**

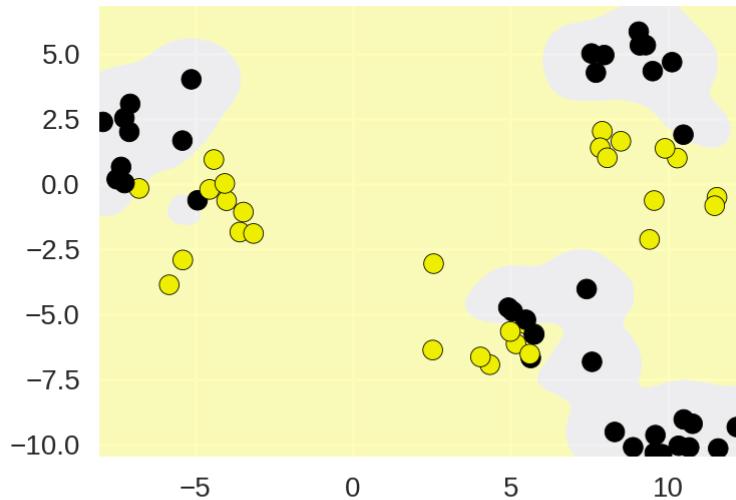
```
In [26]: from adspy_shared_utilities import plot_class_regions_for_classifier

X_train, X_test, y_train, y_test = train_test_split(X_D2, y_D2, random_state = 0)
fig, subaxes = plt.subplots(3, 1, figsize=(4, 11))

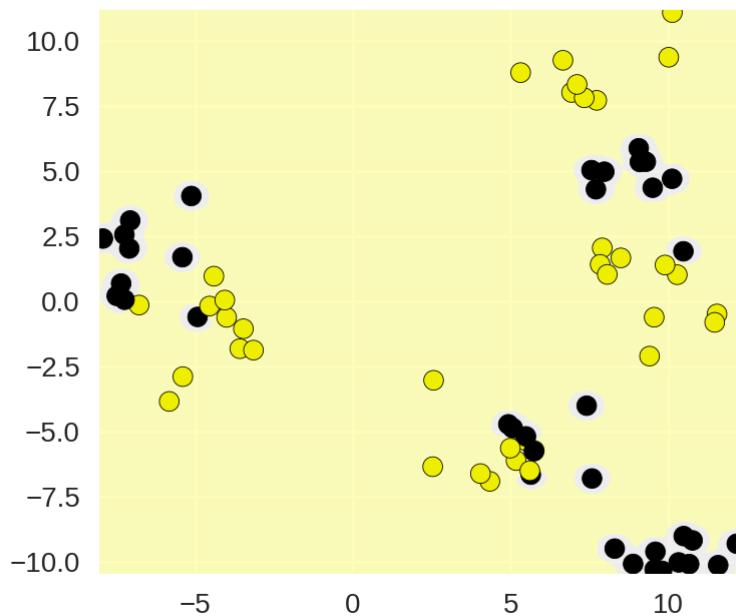
for this_gamma, subplot in zip([0.01, 1.0, 10.0], subaxes):
    clf = SVC(kernel = 'rbf', gamma=this_gamma).fit(X_train, y_train)
    title = 'Support Vector Classifier:\nRBF kernel, gamma = {:.2f}'.format(this_gamma)
    plot_class_regions_for_classifier_subplot(clf, X_train, y_train,
                                              None, None, title, subplot)
plt.tight_layout()
```

Figure 19





Support Vector Classifier:
RBF kernel, gamma = 10.00



Support Vector Machine with RBF kernel: using both C and gamma parameter


```
In [27]: from sklearn.svm import SVC
from adspy_shared_utilities import plot_class_regions_for_classifier_subplot

from sklearn.model_selection import train_test_split

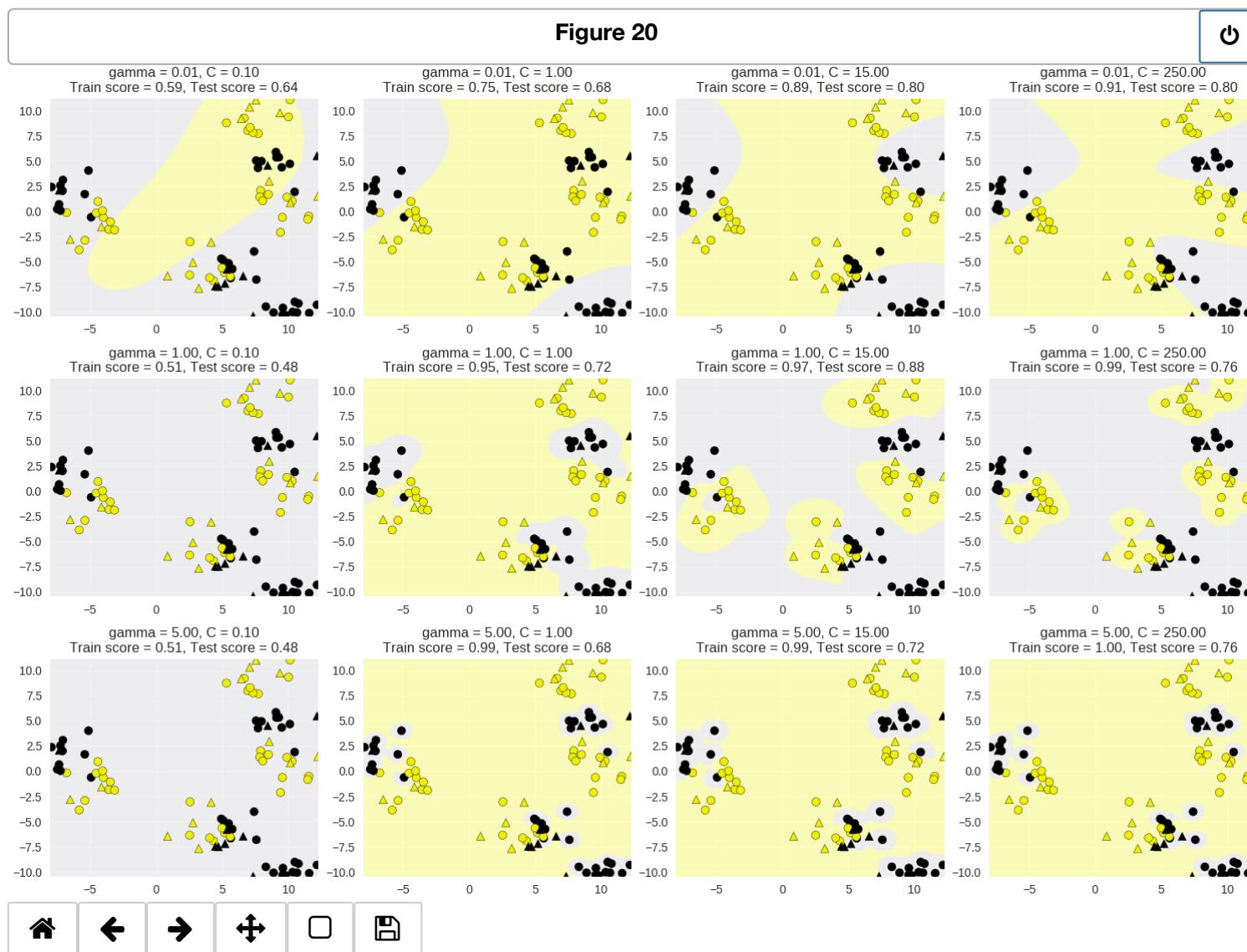
X_train, X_test, y_train, y_test = train_test_split(X_D2, y_D2, random_state = 0)
fig, subaxes = plt.subplots(3, 4, figsize=(15, 10), dpi=50)

for this_gamma, this_axis in zip([0.01, 1, 5], subaxes):

    for this_C, subplot in zip([0.1, 1, 15, 250], this_axis):
        title = 'gamma = {:.2f}, C = {:.2f}'.format(this_gamma, this_C)
        clf = SVC(kernel = 'rbf', gamma = this_gamma,
                   C = this_C).fit(X_train, y_train)
        plot_class_regions_for_classifier_subplot(clf, X_train, y_train,
                                                X_test, y_test, title,
                                                subplot)
plt.tight_layout(pad=0.4, w_pad=0.5, h_pad=1.0)
```



Figure 20



Application of SVMs to a real dataset: unnormalized data

```
In [28]: from sklearn.svm import SVC
X_train, X_test, y_train, y_test = train_test_split(X_cancer, y_cancer,
                                                    random_state = 0)

clf = SVC(C=10).fit(X_train, y_train)
print('Breast cancer dataset (unnormalized features)')
print('Accuracy of RBF-kernel SVC on training set: {:.2f}'
      .format(clf.score(X_train, y_train)))
print('Accuracy of RBF-kernel SVC on test set: {:.2f}'
      .format(clf.score(X_test, y_test)))

Breast cancer dataset (unnormalized features)
Accuracy of RBF-kernel SVC on training set: 1.00
Accuracy of RBF-kernel SVC on test set: 0.63
```

Application of SVMs to a real dataset: normalized data with feature preprocessing using minmax scaling

```
In [29]: from sklearn.preprocessing import MinMaxScaler
scaler = MinMaxScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)

clf = SVC(C=10).fit(X_train_scaled, y_train)
print('Breast cancer dataset (normalized with MinMax scaling)')
print('RBF-kernel SVC (with MinMax scaling) training set accuracy: {:.2f}'
      .format(clf.score(X_train_scaled, y_train)))
print('RBF-kernel SVC (with MinMax scaling) test set accuracy: {:.2f}'
      .format(clf.score(X_test_scaled, y_test)))

Breast cancer dataset (normalized with MinMax scaling)
RBF-kernel SVC (with MinMax scaling) training set accuracy: 0.98
RBF-kernel SVC (with MinMax scaling) test set accuracy: 0.96
```

Cross-validation

Example based on k-NN classifier with fruit dataset (2 features)

```
In [30]: from sklearn.model_selection import cross_val_score

clf = KNeighborsClassifier(n_neighbors = 5)
X = X_fruits_2d.as_matrix()
y = y_fruits_2d.as_matrix()
cv_scores = cross_val_score(clf, X, y)

print('Cross-validation scores (3-fold):', cv_scores)
print('Mean cross-validation score (3-fold): {:.3f}'
     .format(np.mean(cv_scores)))
```

```
Cross-validation scores (3-fold): [ 0.77  0.74  0.83]
Mean cross-validation score (3-fold): 0.781
```

A note on performing cross-validation for more advanced scenarios.

In some cases (e.g. when feature values have very different ranges), we've seen the need to scale or normalize the training and test sets before use with a classifier. The proper way to do cross-validation when you need to scale the data is *not* to scale the entire dataset with a single transform, since this will indirectly leak information into the training data about the whole dataset, including the test data (see the lecture on data leakage later in the course). Instead, scaling/normalizing must be computed and applied for each cross-validation fold separately. To do this, the easiest way in scikit-learn is to use *pipelines*. While these are beyond the scope of this course, further information is available in the scikit-learn documentation here:

<http://scikit-learn.org/stable/modules/generated/sklearn.pipeline.Pipeline.html> (<http://scikit-learn.org/stable/modules/generated/sklearn.pipeline.Pipeline.html>)

or the Pipeline section in the recommended textbook: Introduction to Machine Learning with Python by Andreas C. Müller and Sarah Guido (O'Reilly Media).

Validation curve example

```
In [31]: from sklearn.svm import SVC
from sklearn.model_selection import validation_curve

param_range = np.logspace(-3, 3, 4)
train_scores, test_scores = validation_curve(SVC(), X, y,
                                             param_name='gamma',
                                             param_range=param_range, cv=3)
```

```
In [32]: print(train_scores)
```

```
[[ 0.49  0.42  0.41]
 [ 0.84  0.72  0.76]
 [ 0.92  0.9   0.93]
 [ 1.    1.    0.98]]
```

```
In [33]: print(test_scores)
```

```
[[ 0.45  0.32  0.33]
 [ 0.82  0.68  0.61]
 [ 0.41  0.84  0.67]
 [ 0.36  0.21  0.39]]
```

```
In [34]: # This code based on scikit-learn validation_plot example
# See: http://scikit-learn.org/stable/auto_examples/model_selection/plot_validation_curve.html
plt.figure()

train_scores_mean = np.mean(train_scores, axis=1)
train_scores_std = np.std(train_scores, axis=1)
test_scores_mean = np.mean(test_scores, axis=1)
test_scores_std = np.std(test_scores, axis=1)

plt.title('Validation Curve with SVM')
plt.xlabel('$\gamma$ (gamma)')
plt.ylabel('Score')
plt.ylim(0.0, 1.1)
lw = 2

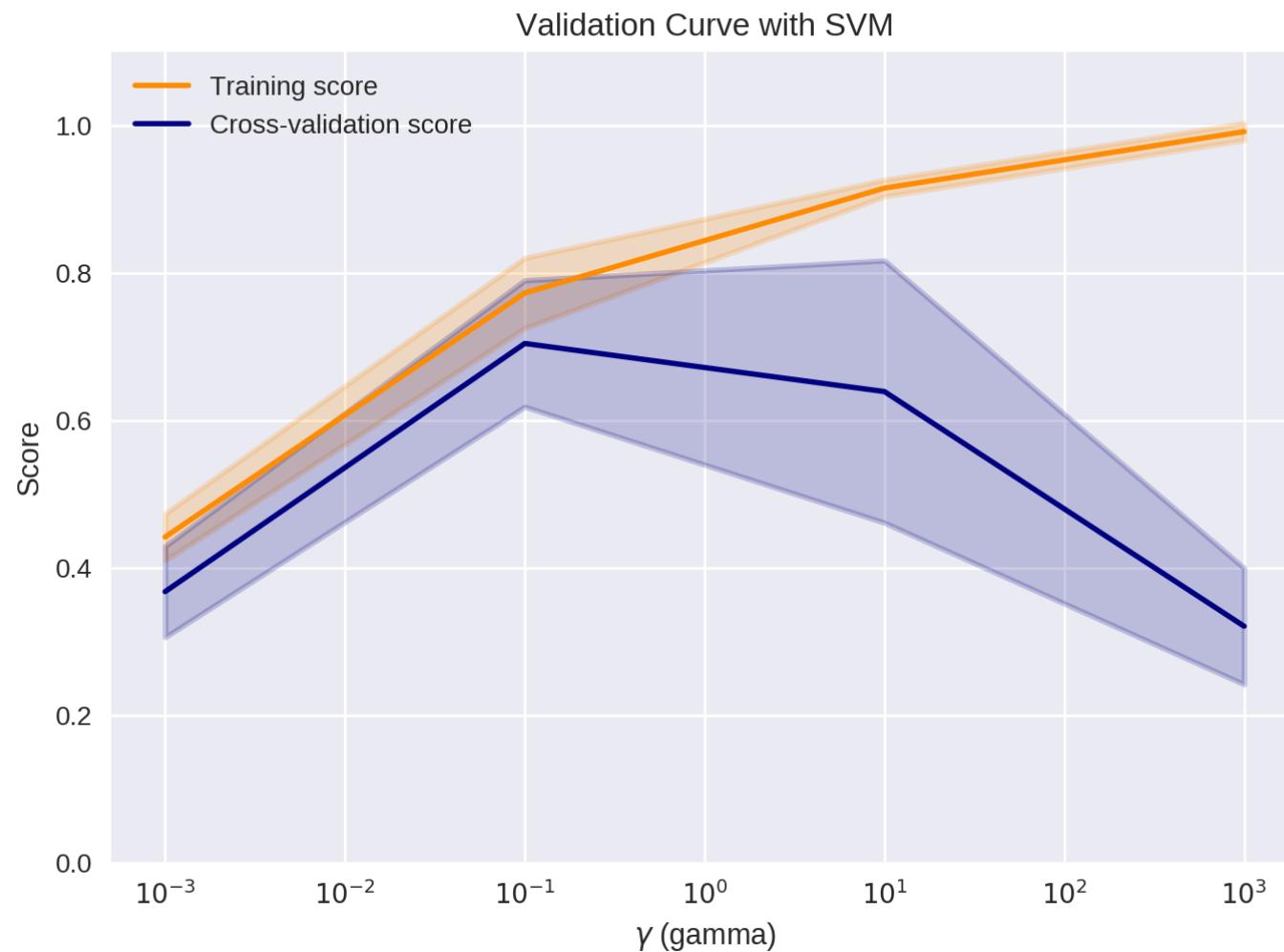
plt.semilogx(param_range, train_scores_mean, label='Training score',
             color='darkorange', lw=lw)

plt.fill_between(param_range, train_scores_mean - train_scores_std,
                 train_scores_mean + train_scores_std, alpha=0.2,
                 color='darkorange', lw=lw)

plt.semilogx(param_range, test_scores_mean, label='Cross-validation score',
             color='navy', lw=lw)

plt.fill_between(param_range, test_scores_mean - test_scores_std,
                 test_scores_mean + test_scores_std, alpha=0.2,
                 color='navy', lw=lw)

plt.legend(loc='best')
plt.show()
```

Figure 21

Decision Trees

```
In [35]: from sklearn.datasets import load_iris
from sklearn.tree import DecisionTreeClassifier
from adspy_shared_utilities import plot_decision_tree
from sklearn.model_selection import train_test_split

iris = load_iris()

X_train, X_test, y_train, y_test = train_test_split(iris.data, iris.target, random_state = 3)
clf = DecisionTreeClassifier().fit(X_train, y_train)

print('Accuracy of Decision Tree classifier on training set: {:.2f}'
     .format(clf.score(X_train, y_train)))
print('Accuracy of Decision Tree classifier on test set: {:.2f}'
     .format(clf.score(X_test, y_test)))
```

Accuracy of Decision Tree classifier on training set: 1.00
Accuracy of Decision Tree classifier on test set: 0.95

Setting max decision tree depth to help avoid overfitting

```
In [36]: clf2 = DecisionTreeClassifier(max_depth = 3).fit(X_train, y_train)

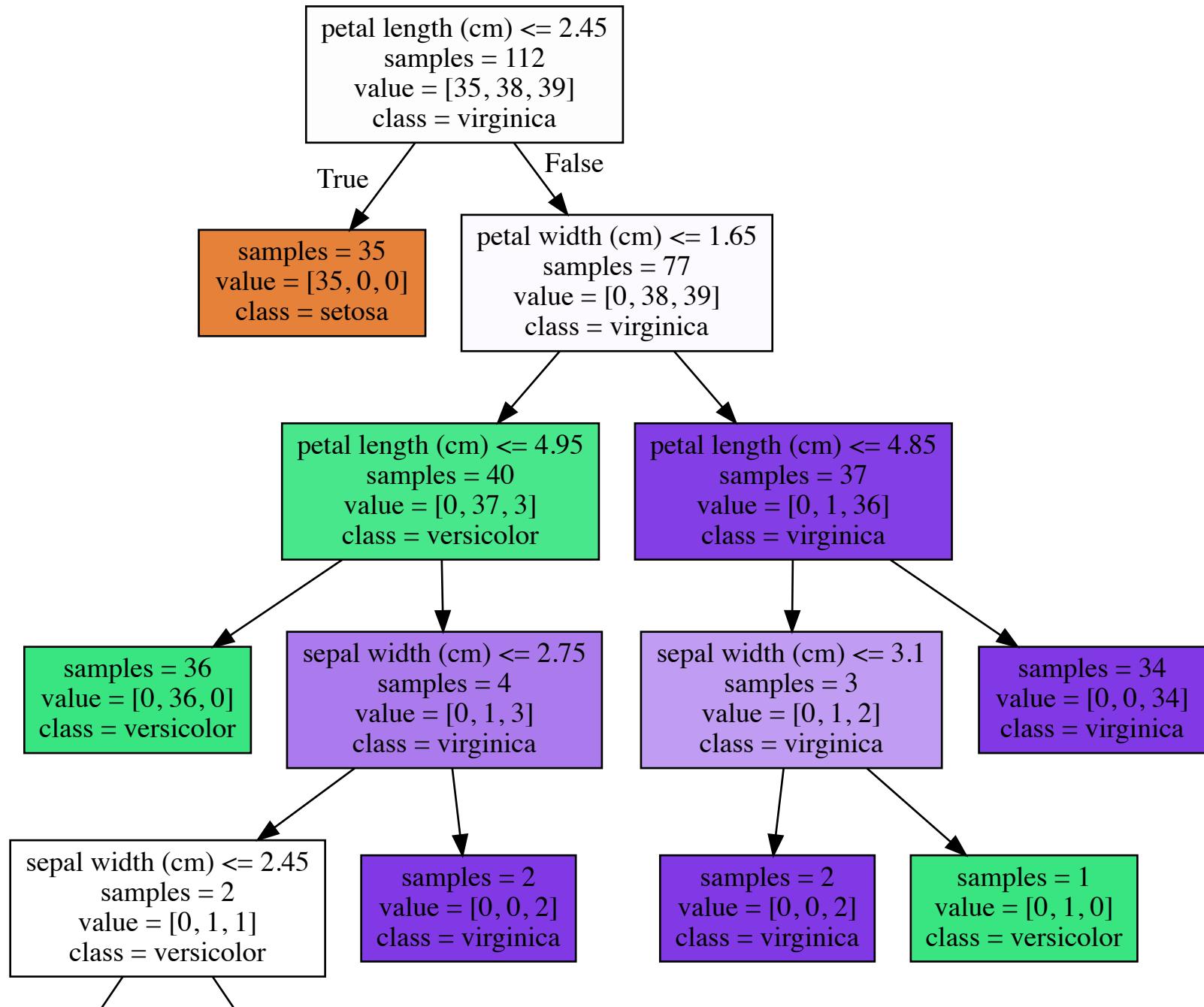
print('Accuracy of Decision Tree classifier on training set: {:.2f}'
     .format(clf2.score(X_train, y_train)))
print('Accuracy of Decision Tree classifier on test set: {:.2f}'
     .format(clf2.score(X_test, y_test)))
```

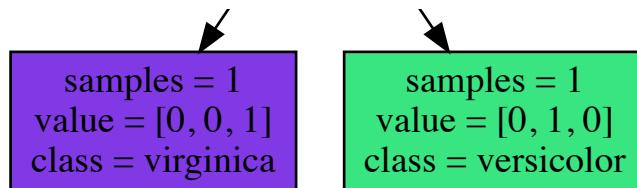
Accuracy of Decision Tree classifier on training set: 0.98
Accuracy of Decision Tree classifier on test set: 0.97

Visualizing decision trees

```
In [37]: plot_decision_tree(clf, iris.feature_names, iris.target_names)
```

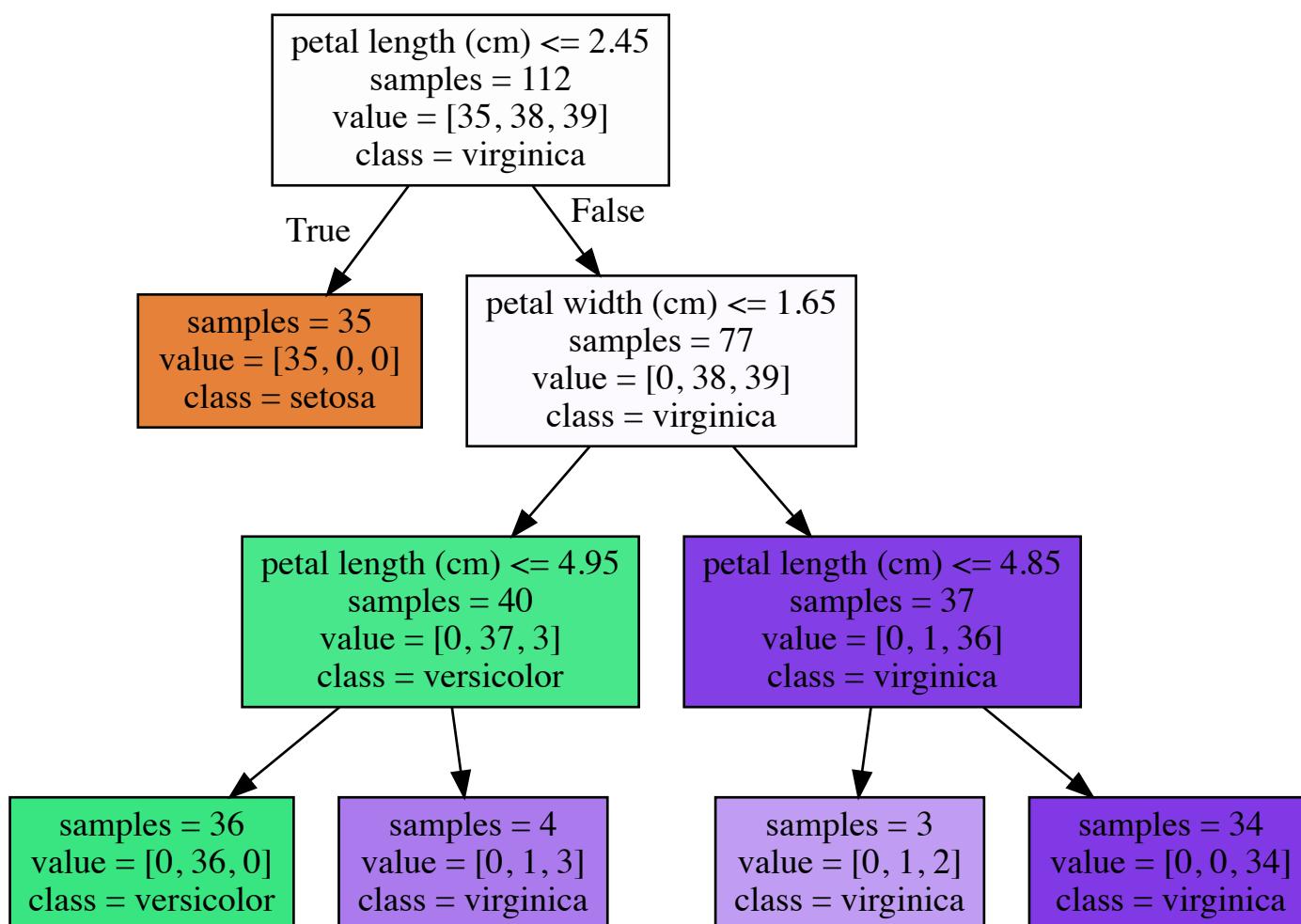
Out[37]:



**Pre-pruned version (max_depth = 3)**

```
In [38]: plot_decision_tree(clf2, iris.feature_names, iris.target_names)
```

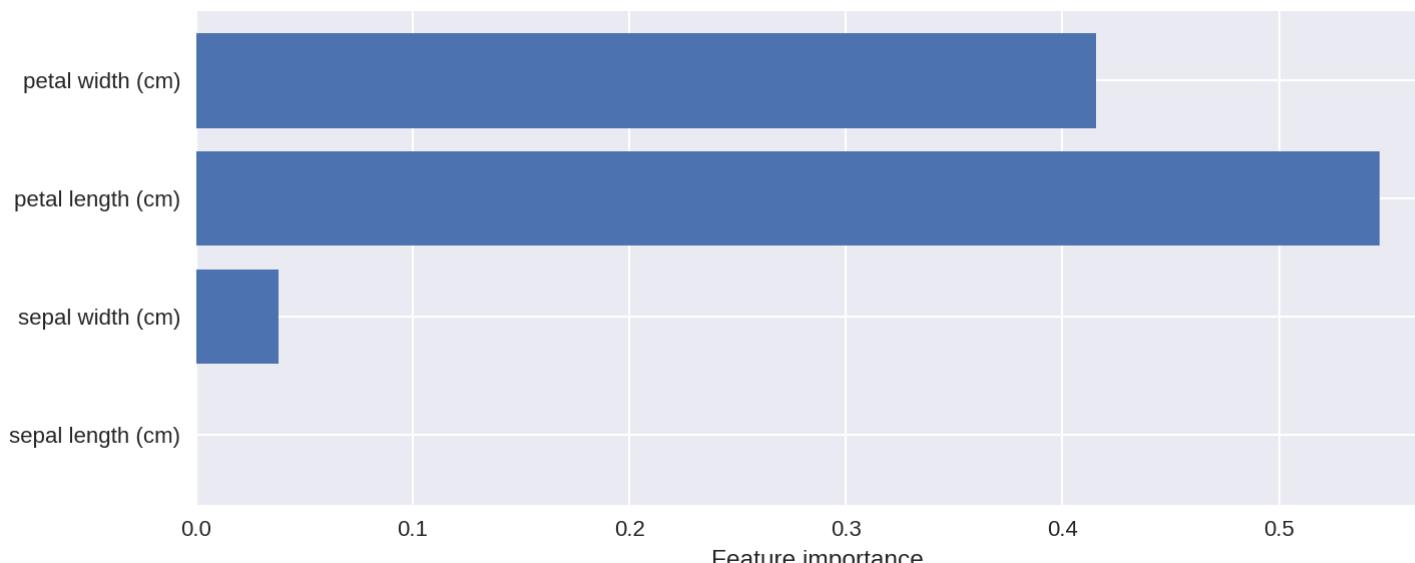
Out[38]:



Feature importance

```
In [39]: from adspy_shared_utilities import plot_feature_importances  
  
plt.figure(figsize=(10,4), dpi=80)  
plot_feature_importances(clf, iris.feature_names)  
plt.show()  
  
print('Feature importances: {}'.format(clf.feature_importances_))
```

Figure 22



Feature importances: [0. 0.04 0.55 0.42]

```
In [40]: from sklearn.tree import DecisionTreeClassifier
from adspy_shared_utilities import plot_class_regions_for_classifier_subplot

X_train, X_test, y_train, y_test = train_test_split(iris.data, iris.target, random_state = 0)
fig, subaxes = plt.subplots(6, 1, figsize=(6, 32))

pair_list = [[0,1], [0,2], [0,3], [1,2], [1,3], [2,3]]
tree_max_depth = 4

for pair, axis in zip(pair_list, subaxes):
    X = X_train[:, pair]
    y = y_train

    clf = DecisionTreeClassifier(max_depth=tree_max_depth).fit(X, y)
    title = 'Decision Tree, max_depth = {:d}'.format(tree_max_depth)
    plot_class_regions_for_classifier_subplot(clf, X, y, None,
                                              None, title, axis,
                                              iris.target_names)

    axis.set_xlabel(iris.feature_names[pair[0]])
    axis.set_ylabel(iris.feature_names[pair[1]])

plt.tight_layout()
plt.show()
```

Figure 23



**Decision Trees on a real-world dataset**

```
In [41]: from sklearn.tree import DecisionTreeClassifier
from adspy_shared_utilities import plot_decision_tree
from adspy_shared_utilities import plot_feature_importances

X_train, X_test, y_train, y_test = train_test_split(X_cancer, y_cancer, random_state = 0)

clf = DecisionTreeClassifier(max_depth = 4, min_samples_leaf = 8,
                             random_state = 0).fit(X_train, y_train)

plot_decision_tree(clf, cancer.feature_names, cancer.target_names)
```

Out[41]:

mean concave points <= 0.0489
samples = 426
value = [159, 267]
class = benign

True / False

```
In [42]: print('Breast cancer dataset: decision tree')
print('Accuracy of DT classifier on training set: {:.2f}'
     .format(clf.score(X_train, y_train)))
print('Accuracy of DT classifier on test set: {:.2f}'
     .format(clf.score(X_test, y_test)))

plt.figure(figsize=(10,6),dpi=80)
plot_feature_importances(clf, cancer.feature_names)
plt.tight_layout()

plt.show()
```

```
Breast cancer dataset: decision tree
Accuracy of DT classifier on training set: 0.96
Accuracy of DT classifier on test set: 0.94
```

Figure 24